Lattice path integral approach to the one-dimensional Kondo model

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Abstract. An integrable Anderson-like impurity model in a correlated host is derived from a gl(2|1)-symmetric transfer matrix by means of the Quantum-Inverse-Scattering-Method (QISM). Using the Quantum Transfer Matrix technique, free energy contributions of both the bulk and the impurity are calculated exactly. As a special case, the limit of a localized moment in a free bulk (Kondo limit) is performed in the Hamiltonian and in the free energy. In this case, high- and low-temperature scales are calculated with high accuracy.

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1. Introduction

Over decades, the model of a localized magnetic impurity in a non-magnetic metal has been one of the major challenges in many-particle theory. Anderson [1] proposed a model of a localized impurity interacting with a host of free electrons through hybridization:

$$H_A = \sum_{k,\tau} \epsilon_k c_{k,\tau}^{\dagger} c_{k,\tau} + \epsilon_d n_d + \sum_{k,\tau} \left(M_k d_{\tau}^{\dagger} c_{k,\tau} + M_k^* c_{k,\tau}^{\dagger} d_{\tau} \right) + U n_{d,\uparrow} n_{d,\downarrow}$$

On the impurity site, a Coulomb repulsion U is allowed. The scattering at the impurity is assumed to be isotropic and therefore one-dimensional. In the limit $|M_k|^2/U \ll 1$, a localized moment forms, which is demonstrated by a canonical transformation of the Anderson model, resulting in the Kondo model [2] with an impurity operator

$$H_i = 2J \sum_{k,k'} c_{k,\tau}^{\dagger} \boldsymbol{\sigma}_{\tau,\tau'} c_{k',\tau'} \boldsymbol{\sigma}_i , \qquad (1)$$

where $\sigma = (\sigma^x, \sigma^y, \sigma^z)$ denotes the Pauli matrices. The Kondo model describes a free host, interacting weakly with a localized magnetic moment via antiferromagnetic XXX spin exchange with an amplitude J. "Weak interaction" means that at high temperatures, the coupling is negligible and the impurity spin shows Curie-Weiss

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behavior. The lesson to be learned from this limit is that a localized moment occurs if singly occupied sites are energetically favourable and hybridization only leads to virtual double or zero occupation. The model (1) served as starting point for Kondo [3], who performed a perturbational calculation of the scattering amplitude between host and impurity up to third order in J. He discovered a $\ln \widetilde{T}_K/T$ contribution to the electrical resistivity. \widetilde{T}_K is the crossover temperature which indicates the limit of perturbation theory: A divergence occurs for $T \sim \widetilde{T}_K$.

The method which overcomes the failure of perturbation theory is scaling. By the implementation of his numerical renormalization group, Wilson [4] achieved a non-perturbative calculation of the impurity contribution to the magnetic susceptibility χ and the specific heat C at $T \ll \tilde{T}_k$. By assuming a linear dispersion in the conduction band he discovered Fermi-liquid-like behavior of the impurity for $T \ll \tilde{T}_K$. In the other extreme, at $T \gg T_K$, Wilson confirmed the asymptotic expansion in $\ln \tilde{T}_K/T$ discovered by perturbation theory techniques.

Andrei [5] and Wiegmann [7] obtained the spectrum exactly by the Bethe Ansatz (BA). The linearized energy-momentum relation turned out to be crucial for the application of the BA. Thermodynamic equilibrium response functions were calculated in the following by employing thermodynamic BA (TBA) techniques, [8]. The impurity contribution to the free energy is encoded in a set of infinitely many coupled NLIE. These contain the whole information about thermodynamic equilibrium functions. Especially, the asymptotic high-temperature expansion due to Kondo and the Wilson ratios are encoded therein. The low temperature Fermi-liquid-like behavior was confirmed in the cited works. However, the high-temperature asymptotic expansion was not performed as far as in Wilson's approach.

We develop a lattice path integral representation of the free energy of a onedimensional Anderson-like impurity model in a correlated host. This model can be viewed as a lattice-regularized version of the Anderson model in the continuum. As a special case, the Kondo model ist obtained in a certain scaling limit. The host is based on a four-dimensional representation of the Lie superalgebra gl(2|1). The corresponding four states per lattice site are zero, single (with spin up or down) and double occupation. The impurity degrees of freedom are described by a three-dimensional representation of gl(2|1). Double occupation on the impurity site is excluded from the beginning. The parameters of the model can be tuned such that on one hand, particle exchange between the impurity site and adjacent host sites is eliminated by a canonical transformation and on the other hand zero occupation is energetically suppressed. The same parameter tuning makes vanish correlations in the host. These conditions fulfilled, a localized moment in a free host occurs (Kondo limit).

In order to regularize the continuous Kondo model, it is quite natural to choose the superalgebra gl(2|1). Its even subalgebra is $u(1) \otimes su(2)$, encoding charge and spin degrees of freedom, respectively. Spin-charge separation occurs in one dimension for interacting electron systems [9], and the impurity is supposed to possess exclusively spin degrees of freedom. Indeed, the scaling limit reduces gl(2|1) to one of its subalgebras,

su(2), in the impurity space. Then the excitation spectrum contains only spin degrees of freedom on the impurity site.

The model proposed in this work allows for the Kondo limit as one special case. We calculate the free energy exactly in the general case, that is an Anderson-like impurity in an interacting host and perform the Kondo limit afterwards. Thus our results are farther reaching than the known non-perturbative treatments of the Kondo model [4, 8]. The free energy of the host and of the impurity are given by eigenvalues of distinct quantum transfer matrices and can therefore be separated. In the Kondo limit, Wilson's results are confirmed with high accuracy. The general Anderson-like case will be investigated elsewhere [10].

This article is organized as follows. In the next section, we derive the Hamiltonian by QISM. The third section deals with the calculation of the free energy. In each of these sections, the Kondo limit is treated explicitly. Section four contains the derivation of Wilson's results in the framework of our path integral approach. A conclusion and an outlook form the last section.

In all what follows we set $k_B = 1$, and $g\mu_B = 1$, where k_B is Boltzmann's constant, g is the gyromagnetic factor and μ_B is the Bohr magneton. An index i (h) denotes quantities pertaining to the impurity (host).

2. The impurity model

Let $V^{(d)}$ be the module giving rise to the d-dimensional irrep of gl(2|1), d = 3, 4. A grading is assigned to the basis vectors through the parity function p,

$$d = 4 : p[1] = p[4] = 0; p[2] = p[3] = 1$$

$$d = 3 : p[1] = p[2] = 0; p[3] = 1.$$
(2)

The matrices $R_{i,j}^{(d,d')}(u) \in \text{End}\left(V_i^{(d)} \otimes V_j^{(d')}\right)$ satisfy the graded Yang-Baxter-Equation (YBE),

$$\begin{aligned}
& \left[R_{2,3}^{(d,d')}(u) \right]_{\beta',\gamma'}^{\beta,\gamma} \left[R_{1,2}^{(d'',d')}(v) \right]_{\alpha',\gamma''}^{\alpha,\gamma'} \left[R_{1,3}^{(d'',d)}(v-u) \right]_{\alpha'',\beta''}^{\alpha',\beta'} (-1)^{(p[\alpha]+p[\alpha'])p[\beta']} \\
& = \left[R_{1,3}^{(d'',d)}(v-u) \right]_{\alpha',\beta'}^{\alpha,\beta} \left[R_{1,2}^{(d'',d')}(v) \right]_{\alpha'',\gamma'}^{\alpha',\gamma} \left[R_{2,3}^{(d,d')}(u) \right]_{\beta'',\gamma''}^{\beta',\gamma'} (-1)^{(p[\alpha']+p[\alpha''])p[\beta']} .
\end{aligned} (3)$$

Summation over doubly occurring indices is implied in the foregoing equation and in all what follows.

Explicit expressions of the R matrices are given in the following,

$$R^{(3,3)}(u) = \frac{1}{u+1} \left(u + (-1)^{p[a]p[b]} e_a^b \otimes e_b^a \right) \tag{4}$$

$$R^{(3,4)}(u) = \frac{1}{u + \frac{\alpha}{2} + 1} \left(u + \frac{\alpha}{2} + 1 + (-1)^{p[a]p[b]} e_a^b \otimes E_b^a \right)$$
 (5)

$$R^{(4,4)}(u) = -\left(1 + \frac{2\alpha}{u - \alpha}\check{P}_1 - \frac{2\alpha + 2}{u + \alpha + 1}\check{P}_3\right). \tag{6}$$

 $e_a^b \; (E_a^b)$ are the nine three- (four-) dimensional generators of gl(2|1), obeying

$$[e_b^a, e_d^c]_{\pm} := e_b^a e_d^c - (-1)^{(p[a]+p[b])(p[c]+p[d])} e_d^c e_b^a$$

$$= \delta_d^a e_b^c - (-1)^{(p[a]+p[b])(p[c]+p[d])} \delta_b^c e_d^a , \qquad (7)$$

and the same for the E_b^a . \check{P}_1 , \check{P}_3 are projectors from $V^{(4)} \otimes V^{(4)}$ onto gl(2|1) modules with highest weights $(0,0|2\alpha)$ and $(-1,-1|2\alpha+2)$ respectively. They are given explicitly in [11]. For a matrix representation of e_b^a , choose the basis

$$|\overline{1}\rangle = (1,0,0) , |\overline{2}\rangle = (0,1,0) , |\overline{3}\rangle = (0,0,1) .$$

Then $e_b^a := |\overline{b}\rangle\langle \overline{a}|$ is the usual matrix representation of projectors in three dimensional space.

As to the E_b^a , we choose a basis in $V^{(4)}$,

$$|1\rangle = (1,0,0,0)$$
, $|2\rangle = (0,1,0,0)$, $|3\rangle = (0,0,1,0)$, $|4\rangle = (0,0,0,1)$.

We call the projectors associated with these states $m_b^a := |b\rangle\langle a|, a, b = 1, 2, 3, 4$. One verifies that the set [11]

$$\begin{split} E_1^1 &= -|3\rangle\langle 3| - |4\rangle\langle 4|, \qquad E_2^2 &= -|2\rangle\langle 2| - |4\rangle\langle 4|, \\ E_3^3 &= \alpha|1\rangle\langle 1| + (\alpha+1)(|2\rangle\langle 2| + |3\rangle\langle 3|) + (\alpha+2)|4\rangle\langle 4|, \\ E_1^2 &= |2\rangle\langle 3|, \qquad E_2^1 &= |3\rangle\langle 2|, \\ E_2^3 &= \sqrt{\alpha}|1\rangle\langle 2| + \sqrt{\alpha+1}|3\rangle\langle 4|, \qquad E_3^2 &= \sqrt{\alpha}|2\rangle\langle 1| + \sqrt{\alpha+1}|4\rangle\langle 3|, \\ E_1^3 &= -\sqrt{\alpha}|1\rangle\langle 3| + \sqrt{\alpha+1}|2\rangle\langle 4|, \qquad E_3^1 &= -\sqrt{\alpha}|3\rangle\langle 1| + \sqrt{\alpha+1}|4\rangle\langle 2| \end{split}$$

satisfies eq. (7). In the sequel, the real parameter α is restricted to $\alpha > 0$.

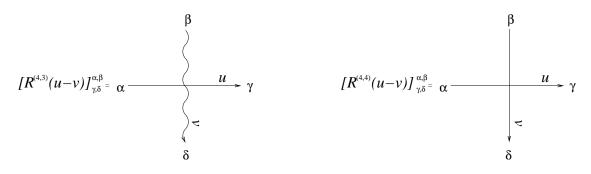
Consider the set of matrices \overline{R} defined by

$$\left[\overline{R}^{(d',d)}(u)\right]_{\gamma,\delta}^{\alpha,\beta} = (-1)^{p[\delta](p[\gamma]+p[\alpha])} \left[R^{(d',d)}(-u)\right]_{\alpha,\delta}^{\gamma,\beta} . \tag{9}$$

The permutation of the indices means that creators and annihilators are exchanged in the auxiliary space of R. These \overline{R} -matrices satisfy

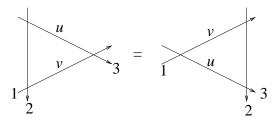
$$\begin{split}
& \left[\overline{R}^{(d,d')}(u) \right]_{\beta',\gamma'}^{\beta,\gamma} \left[\overline{R}^{(d'',d')}(v) \right]_{\alpha',\gamma''}^{\alpha,\gamma'} \left[R^{(d'',d)}(v-u) \right]_{\alpha'',\beta''}^{\alpha',\beta'} (-1)^{(p[\alpha]+p[\alpha'])p[\beta']} \\
&= \left[R^{(d'',d)}(v-u) \right]_{\alpha',\beta'}^{\alpha,\beta} \left[\overline{R}^{(d'',d')}(v) \right]_{\alpha'',\gamma''}^{\alpha',\gamma'} \left[\overline{R}^{(d,d')}(u) \right]_{\beta'',\gamma''}^{\beta',\gamma'} (-1)^{(p[\alpha']+p[\alpha''])p[\beta']} .
\end{split}$$
(10)

The R-matrices can be translated into a graphical language. Straight lines denote the 4-dimensional space, wavy lines symbolize three-dimensional space,



The two lines symbolize the two spaces intertwined by $R_{i,j}$. Each line carries a direction indicated by an arrow; both the vertical and horizontal lines carry spectral parameters. The argument of R is given by the difference between the right and the left "incoming" parameters. The replacement $R \to \overline{R}$ means flipping the arrow on the vertical bond.

The YBE eq. (3) in graphical language reads:



"Other" YBEs are obtained by flipping arrows (that means replacing $R \to \overline{R}$) and/or substituting straight by wavy lines (that is, changing the dimension in one of the spaces).

"Unitarity" is a further property of the R-matrices.

$$\left[R^{(d,d')}(u)\right]_{\delta,\alpha}^{\beta,\gamma} \left[R^{(d',d)}(-u)\right]_{\gamma',\beta'}^{\alpha,\delta} = \delta_{\beta'}^{\beta} \delta_{\gamma'}^{\gamma} , \qquad (11)$$

and the same for \overline{R} . The unitarity property fixes normalization constants of the R-matrices. In the following, we will speak of "normalized" R-matrices when they satisfy eq. (11); non-normalized R-matrices differ from those by constant pre-factors, but still fulfill the YBE. A direct verification of eq. (11) for d = d' = 3 (d = d' = 4) is done by using the projection properties

$$e_b^a e_d^c = \delta_d^a e_b^c, \, \check{P}_j \check{P}_k = \delta_{j,k} \check{P}_k, \qquad (12)$$

or by using the YBE with standard initial conditions. Furthermore, for d = 3, d' = 4 in eq. (11), one should employ

$$E^{\alpha}_{\beta} E^{\beta}_{\delta}(-1)^{p[\beta](p[\alpha]+p[\delta])} = -(\alpha+2)(-1)^{p[\alpha]p[\delta]} E^{\alpha}_{\delta}.$$

In order to construct a lattice model, one embeds m_a^b , e_a^b into $\operatorname{End}\left[V^{(3)}\otimes\left(V^{(4)}\right)^{\otimes L}\right]$, such that e_a^b acts non-trivially only on the lattice site 0. Therefore consider the graded tensor product of two operators v, w:

$$v_b^a \otimes_s w_d^c = (-1)^{(p[a]+p[b])p[d]} v_b^a \otimes w_d^c$$
,

where v, w stand for e, m. The operator of unity in three- (four-)dimensional space is $I_3 = e_c^c (I_4 = m_c^c)$. Following [12], define

$$[e_{0}]_{b}^{a} := e_{b}^{a} \otimes_{s} I_{4}^{\otimes_{s}L}$$

$$= (-1)^{(p[a]+p[b])\sum_{k=1}^{L} p[c_{k}]} e_{b}^{a} \otimes m_{c_{1}}^{c_{1}} \otimes \cdots \otimes m_{c_{L}}^{c_{L}}$$

$$[m_{j}]_{b}^{a} := I_{3} \otimes_{s} I_{4}^{\otimes_{s}(j-1)} \otimes_{s} m_{b}^{a} \otimes_{s} I_{4}^{\otimes_{s}(L-j)}$$

$$= (-1)^{(p[a]+p[b])\sum_{k=j+1}^{L} p[c_{k}]} I_{3} \otimes I_{4}^{\otimes(j-1)} m_{b}^{a} \otimes m_{c_{1}}^{c_{1}} \otimes \cdots \otimes m_{c_{L}}^{c_{L}},$$

with $j = 1, \ldots, L$. Then

$$[e_0]_b^a [e_0]_d^c = \delta_d^a [e_0]_b^c \tag{13a}$$

$$[e_0]_b^a [m_k]_d^c = (-1)^{(p[a]+p[b])(p[c]+p[d])} [m_k]_d^c [e_0]_b^a.$$
(13b)

Analogous relations hold between m_i , m_k .

Principally, at this point one could derive the Hamiltonian. However, it is more convenient to find a fermionic representation of the R matrices in order to use the more familiar language of fermionic field operators $c_{\tau,j}^{\dagger}, c_{\tau,j}$, acting on the spin directions $\tau = \uparrow, \downarrow$ and on the lattice site j. This is done by employing the technique of Göhmann [12, 13], which consists in identifying the $[m_j]_b^a$, $[e_0]_b^a$ with certain combinations of fermionic operators.

The entries $[X_j]_b^a$ of the matrix

$$X_{j} = \begin{pmatrix} n_{j\downarrow}n_{j\uparrow} & n_{j\downarrow}c_{j\uparrow}^{\dagger} & c_{j\downarrow}^{\dagger}n_{j\uparrow} & c_{j\downarrow}^{\dagger}c_{j\uparrow}^{\dagger} \\ n_{j\downarrow}c_{j\uparrow} & n_{j\downarrow}(1-n_{j\uparrow}) & -c_{j\downarrow}^{\dagger}c_{j\uparrow} & -c_{j\downarrow}^{\dagger}(1-n_{j\uparrow}) \\ c_{j\downarrow}n_{j\uparrow} & c_{j\downarrow}c_{j\uparrow}^{\dagger} & (1-n_{j\downarrow})n_{j\uparrow} & (1-n_{j\downarrow})c_{j\uparrow}^{\dagger} \\ -c_{j\downarrow}c_{j\uparrow} & -c_{j\downarrow}(1-n_{j\uparrow}) & (1-n_{j\downarrow})c_{j\uparrow} & (1-n_{j\downarrow})(1-n_{j\uparrow}) \end{pmatrix}$$
(14)

satisfy projection and commutation properties formally identical to eqs. (13a), (13b) with grading p[1] = p[4] = 0, p[2] = p[3] = 1 in accordance with eq. (2) for d = 4. This is the only constraint on $[m_j]_b^a$, so that we identify $[X_j]_b^a \equiv [m_j]_b^a$. The whole set (8) reads in fermionic language:

$$\begin{split} &[E_{j}]_{3}^{3} = \alpha + 2 - (n_{j\downarrow} + n_{j\uparrow}) \\ &[E_{j}]_{1}^{1} = n_{j\downarrow} - 1 & [E_{j}]_{2}^{2} = n_{j\uparrow} - 1 \\ &[E_{j}]_{3}^{1} = -c_{j\uparrow}^{\dagger} c_{j\downarrow} & [E_{j}]_{1}^{2} = -c_{j\downarrow}^{\dagger} c_{j\uparrow} \\ &[E_{j}]_{3}^{1} = -\sqrt{\alpha} \, n_{j\uparrow} c_{j\downarrow} - \sqrt{\alpha + 1} \, (1 - n_{j\uparrow}) c_{j\downarrow} & [E_{j}]_{1}^{3} = -\sqrt{\alpha} \, n_{j\uparrow} c_{j\downarrow}^{\dagger} - \sqrt{\alpha + 1} \, (1 - n_{j\uparrow}) c_{j\downarrow}^{\dagger} \\ &[E_{j}]_{3}^{2} = \sqrt{\alpha} \, n_{j\downarrow} c_{j\uparrow} - \sqrt{\alpha + 1} \, (1 - n_{j\downarrow}) c_{j\uparrow} & [E_{j}]_{2}^{3} = \sqrt{\alpha} \, n_{j\downarrow} c_{j\uparrow}^{\dagger} - \sqrt{\alpha + 1} \, (1 - n_{j\downarrow}) c_{j\uparrow}^{\dagger} \end{split}$$

The even sub-algebras are manifest: E_3^3 is the u(1)-generator, and $E_{1,2}^{1,2}$ are the su(2) generators. The fermionization of the three-dimensional e_b^a is done with the matrix Y, resulting from X, eq. (14) by deleting the first row and column,

$$Y = \begin{pmatrix} n_{d,\downarrow}(1 - n_{d,\uparrow}) & -d_{\downarrow}^{\dagger}d_{\uparrow} & -d_{\downarrow}^{\dagger}(1 - n_{d,\uparrow}) \\ d_{\downarrow}d_{\uparrow}^{\dagger} & (1 - n_{d,\downarrow})n_{d,\uparrow} & (1 - n_{d,\downarrow})d_{\uparrow}^{\dagger} \\ -d_{\downarrow}(1 - n_{d,\uparrow}) & (1 - n_{d,\downarrow})d_{\uparrow} & (1 - n_{d,\downarrow})(1 - n_{d,\uparrow}) \end{pmatrix} . \tag{15}$$

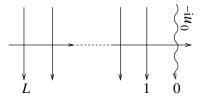
We slightly modified the notation, replacing c^{\dagger} , c, n by d^{\dagger} , d, n_d . Horizontal and vertical bars separate fermionic and bosonic sectors. The boxes on the diagonal of Y contain the generators of su(2), u(1). Set $[e_0]_a^b = Y_a^b$, such that eqs. (13a), (13b) hold with grading $\{1, 1, 0\}$.

The monodromy matrices

$$T(u) = R_{a,L}^{(4,4)}(u)R_{a,L-1}^{(4,4)}(u) \dots R_{a,1}^{(4,4)}(u)R_{a,0}^{(4,3)}(u+iu_0)$$

$$\overline{T}(u) = \overline{R}_{a,L}^{(4,4)}(-u)\overline{R}_{a,L-1}^{(4,4)}(-u) \dots \overline{R}_{a,1}^{(4,4)}(-u)\overline{R}_{a,0}^{(4,3)}(-u+iu_0)$$
(16)

consist of sequences of R matrices, multiplied in (horizontal) auxiliary space. Note the shift by iu_0 on the zeroth lattice site, where the dimension of the (vertical) quantum space is reduced by one. This site shall be denoted as "impurity site". The shift is done by $iu_0 \in \mathbb{C}$, for reasons which will become clear later. Graphically, T(u) is depicted as



The super-trace is called transfer matrix

$$\tau(u) = \operatorname{str}_a T(u) , \qquad \overline{\tau}(u) = \operatorname{str}_a \overline{T}(u)$$
 (17)

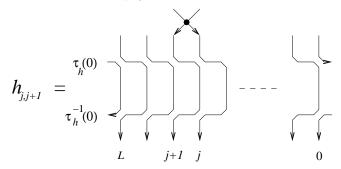
$$\ln\left[\tau\overline{\tau}\right](u) = \ln\left[\tau\overline{\tau}\right](0) + u\underbrace{\left[\tau^{-1}(0)\tau'(u) + \overline{\tau}^{-1}(0)\overline{\tau}'(u)\right]_{u=0}}_{=: \text{ const.}H} + O(u^2) . \quad (18)$$

In the last line, the Hamiltonian was defined as the logarithmic derivative of the two transfer matrices at zero spectral parameter. By scaling u, one is free to multiply the Hamiltonian by a constant factor.

Before evaluating eq. (18), let us shortly comment on the case of a homogeneous model without impurity. We denote the corresponding quantities with a subscript h. This model has been extensively studied in [11, 17]. Assuming periodic boundary conditions $1 \equiv L + 1$, $\tau_h(0)$ ($\overline{\tau}_h(0)$) is the right (left) shift operator, and

$$\ln \tau_h(0) = iP = -\ln \overline{\tau}_h(0) , \qquad (19)$$

where P is the generator of translations to the right. The derivative with respect to u in eq. (18) yields a sum of L terms, each one corresponding to $R'_{j,j+1}(0)$, $j=1,\ldots,L$. For the ease of notation, let us follow the graphical depiction of [16]. The following figure shows the jth term of $\left[\tau_h^{-1}(0)\tau'_h(u)\right]_{u=0}$:



The vertex with a dot denotes $R'_{j,j+1}(0)$. For u=0, the vertices decouple and taking the trace over a row yields the right shift operator $\tau_h(0)$. Thus

$$H_h = \sum_{j=1}^{L} h_{j,j+1} \tag{20}$$

$$h_{j,j+1} = (\alpha + 1)D \frac{\mathrm{d}}{\mathrm{d}u} \ln \left[R^{(4,4)}(u) \right]_{j,j+1;u=0}$$

 H_h is scaled by $D(\alpha + 1)$, D is a bandwidth parameter whose significance will become clear later. Using explicit expressions for $R_{j,j+1}^{(4,4)}$ from [11] one confirms the expression for $h_{j,j+1}$ given in [17]:

$$h_{j,j+1} = (\alpha + 1)D\left(\frac{2}{\alpha}(\check{P}_1)_{j,j+1} - \frac{2}{\alpha + 1}(\check{P}_3)_{j,j+1}\right)$$

$$= -D \sum_{\tau} (c_{j,\tau}^{\dagger} c_{j+1,\tau} + c_{j+1,\tau}^{\dagger} c_{j,\tau}) e^{-\frac{\eta}{2} (n_{j,\overline{\tau}} + n_{j+1,\overline{\tau}})}$$

$$+ U (n_{j,\uparrow} n_{j,\downarrow} + n_{j+1,\uparrow} n_{j+1,\downarrow}) + t_p \left(c_{j+1,\uparrow}^{\dagger} c_{j+1,\downarrow}^{\dagger} c_{j,\uparrow} c_{j,\downarrow} + c_{j,\uparrow}^{\dagger} c_{j,\downarrow}^{\dagger} c_{j+1,\uparrow} c_{j+1,\downarrow} \right)$$

$$+ D(n_j + n_{j+1}) - 2D , \qquad (21)$$

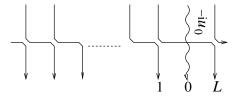
$$U = \frac{D}{\alpha} = t_p , e^{-\eta} = \frac{\alpha + 1}{\alpha} ; \overline{\tau} = -\tau .$$

One can show by a canonical transformation [17] that the limit $\alpha \to 0$ leads to the t-J-model. On the other hand, for $\alpha \gg 1$, the leading order are free fermions:

$$H_{h}/D = 2\sum_{j=1}^{L} n_{j} - 2 - \sum_{j=1}^{L} \sum_{\tau} \left(c_{j,\tau}^{\dagger} c_{j+1,\tau} + c_{j+1,\tau}^{\dagger} c_{j,\tau} \right) \left[1 + \frac{1}{2\alpha} (n_{j,\bar{\tau}} + n_{j+1,\bar{\tau}}) \right] + \frac{2}{\alpha} \sum_{j=1}^{L} n_{j,\uparrow} n_{j,\downarrow} + \frac{1}{\alpha} \sum_{j=1}^{L} \left(c_{j+1,\uparrow}^{\dagger} c_{j+1,\downarrow}^{\dagger} c_{j,\uparrow} c_{j,\downarrow} + c_{j,\uparrow}^{\dagger} c_{j,\downarrow}^{\dagger} c_{j+1,\uparrow} c_{j+1,\downarrow} \right) + O\left(D/\alpha^{3/2}\right). (22)$$

Since in this work, we aim at realizing a free host, our interest is in the limit $\alpha \gg 1$.

Due to the insertion of $R_{a,0}^{(4,3)}$, H receives an impurity contribution H_i . It can be derived graphically. First observe that eq. (19) no longer holds; but due to unitarity (11), one still has $\tau(0) = \overline{\tau}^{-1}(0)$. Then $\tau(0)$ is depicted as:



In comparison with the free host, the changes induced by the impurity stemming from $\ln \tau'(0)$ correspond to the graphs:



A vertex with a dot symbolizes the derivative with respect to the spectral parameter. The first term,

$$R_{1,0}^{(3,4)}(-\mathrm{i}u_0) \left[R_{1,0}^{(4,3)} \right]' (\mathrm{i}u_0) = R_{1,0}^{-1}{}^{(4,3)}(\mathrm{i}u_0) \left[R_{1,0}^{(4,3)} \right]' (\mathrm{i}u_0) ,$$

couples the impurity to the left neighboring site. The second term,

$$R_{1,0}^{(3,4)}(-\mathrm{i}u_0)\frac{h_{L,1}}{D(\alpha+1)}R_{1,0}^{(4,3)}(\mathrm{i}u_0) = R_{1,0}^{-1}{}^{(4,3)}(\mathrm{i}u_0)\frac{h_{L,1}}{D(\alpha+1)}R_{1,0}^{(4,3)}(\mathrm{i}u_0)\;,$$

is a three site coupling. Analogous terms, with L and 1 interchanged, are provided by $\ln \overline{\tau}'(0)$. The inverse matrix $\left[R^{(4,3)}\right]^{-1}$ is found by eq. (11). In analogy to the host Hamiltonian, the spectral parameter u is scaled by $D(\alpha + 1)$, where D is a bandwidth

parameter. Using the fermionization technique, we calculate H_i . It contains terms which are symmetric and others which are antisymmetric under $(L \leftrightarrow 1)$ exchange. In the combined thermodynamic and continuum limit, the latter do not interact with the impurity [18], so we do not consider them in the following. Then

$$H_{i} = -2DJ_{\alpha}(1 - n_{d}) \left(\alpha + F_{1,L}\right) \mathcal{P}_{d}$$

$$- DJ_{\alpha} \sqrt{\alpha} \mathcal{P}_{d} \sum_{\tau} \left[d_{\tau}^{\dagger}(c_{L,\tau} + c_{1,\tau}) - d_{\tau}(c_{L,\tau}^{\dagger} + c_{1,\tau}^{\dagger}) \right] \mathcal{P}_{d}$$

$$+ DJ_{\alpha} \sum_{\tau} n_{d,\tau} \left(c_{L,\tau}^{\dagger} c_{1,\tau} + c_{1,\tau}^{\dagger} c_{L,\tau} \right) \mathcal{P}_{d}$$

$$+ DJ_{\alpha} \sum_{\tau} d_{\tau}^{\dagger} d_{\bar{\tau}} \left(c_{L,\bar{\tau}}^{\dagger} c_{1,\tau} + c_{1,\bar{\tau}}^{\dagger} c_{L,\tau} \right) \mathcal{P}_{d} + O\left(DJ_{\alpha}/\alpha^{1/2}\right) , \qquad (23)$$

where the projector $\mathcal{P}_d := 1 - n_{d,\uparrow} n_{d,\downarrow}$ projects onto non-doubly occupied states on the impurity site. Furthermore,

$$F_{1,L} = 2 - 2\hat{h} - c_{1,\uparrow}^{\dagger} c_{L,\uparrow} - c_{1,\downarrow}^{\dagger} c_{L,\downarrow} - c_{L,\uparrow}^{\dagger} c_{1,\uparrow} - c_{L,\downarrow}^{\dagger} c_{1,\downarrow}$$

$$J_{\alpha} = \frac{2\alpha}{v_0^2 + \alpha^2} > 0 , v_0 := u_0/2$$
(24)

with the most interesting range of the coupling constant

$$\alpha^{-2} \lesssim J_{\alpha} \lesssim \alpha^{-1}$$
 (25)

In Appendix A, an alternative fermionization is used, resulting in essentially the same Hamiltonian.

Finally, one includes external fields μ , h, by

$$H_{ex} = \frac{h}{2} \left[\sum_{j=1}^{L} (n_{j,\uparrow} - n_{j,\downarrow}) + (n_{d,\uparrow} - n_{d,\downarrow}) \right] - \mu \left[\sum_{j=1}^{L} n_j + n_d \mathcal{P}_d \right] . \tag{26}$$

Eqs. (22), (23), (26) define the entire Hamiltonian of the impurity model in the limit of an asymptotically free host. In Appendix B, it is shown that $H_h + H_i$ displays gl(2|1) symmetry. H_{ex} breaks this symmetry, but preserves integrability.

The Kondo limit can be performed by a canonical transformation which eliminates transitions between single and zero occupation of the impurity site. It is conveniently done in Fourier space:

$$c_{j,\tau}^{\dagger} = \frac{1}{\sqrt{L}} \sum_{k=-\pi}^{\pi} c_{k,\tau}^{\dagger} e^{ikj}$$

$$H_{h} = D \left\{ \sum_{k} \sum_{\tau} \epsilon_{k} c_{k,\tau}^{\dagger} c_{k,\tau} - 2 + \frac{2}{L \alpha} \sum_{Q,q,q'} \left[\sum_{\tau} \cos \frac{Q}{2} \cos \left(q + \frac{Q}{2} \right) c_{q+Q,\tau}^{\dagger} c_{q,\tau} c_{q'-Q,\bar{\tau}}^{\dagger} c_{q',\bar{\tau}} + c_{q,\uparrow}^{\dagger} c_{q+Q,\uparrow} c_{q'-Q,\downarrow}^{\dagger} c_{q',\downarrow} - \cos(q+q') c_{q+Q,\uparrow}^{\dagger} c_{q,\uparrow} c_{q,\uparrow} c_{q'-Q,\downarrow}^{\dagger} c_{q',\downarrow} \right] \right\}$$

$$\epsilon_{k} = 2(\cos k + 1) - \mu/D$$
(28)

$$H_{i} = \{2DJ_{\alpha}(n_{d} - 1)(\alpha + F_{1,L}) - \mu n_{d}\} \mathcal{P}_{d} + J_{\alpha}(\alpha D)^{1/2} \mathcal{P}_{d} \sum_{k,\tau} (M_{k} d_{\tau}^{\dagger} c_{k,\tau} + M_{k}^{*} c_{k,\tau}^{\dagger} d_{\tau}) \mathcal{P}_{d} + J_{\alpha} \sum_{\tau,k,k'} N_{k,k'} \left[n_{d,\tau} c_{k,\tau}^{\dagger} c_{k',\tau} + d_{\tau}^{\dagger} d_{\bar{\tau}} c_{k,\bar{\tau}}^{\dagger} c_{k',\tau} \right] \mathcal{P}_{d}$$

$$M_{k} = -\frac{1}{\sqrt{l}} \left(1 + e^{ik} \right) , N_{k,k'} = \frac{1}{l} \left(e^{-ik'} + e^{ik} \right) .$$
(29)

Here l = L/D is the constant length of the chain, and D^{-1} plays the role of a lattice constant. The canonical transformation is generated by an operator A, which yields a transformed Hamiltonian $H_{eff} = \exp(A)H \exp(-A)$ not containing any hybridization between impurity and host in the leading order $O(J_{\alpha})$. One verifies that

$$A = J_{\alpha} \sqrt{\frac{\alpha}{D}} \mathcal{P}_d \sum_{k,\tau} \frac{1}{\epsilon_d - \epsilon_k} (M_k d_{\tau}^{\dagger} c_{k,\tau} - M_k^* c_{k,\tau}^{\dagger} d_{\tau}) \mathcal{P}_d , \qquad (30)$$

where $\epsilon_d := 2J_{\alpha}\alpha n_d - \mu/D$ has been defined. H_{eff} contains terms $O(\alpha J_{\alpha}^2)$. Given the restriction (25), these terms can be neglected. After the transformation, the excitation spectrum of the impurity site contains only the contribution for single occupation. The contribution for non-occupation in the impurity operator is energetically suppressed in the strong coupling limit: In the language of renormalization theory, v_0 drives the impurity Hamiltonian to a strong coupling fixed point at low temperatures. This will be demonstrated in the next section. Thus we do not consider the contribution from zero occupation to the Hamiltonian in the ongoing.

To perform the scaling limit, the fermionic spectrum is linearized around incommensurate Fermi points $\pm k_F$ avoiding Umklapp scattering. The linearization gives rise to right (left) moving particles R (L). To avoid divergences due to the unbounded linear spectrum, operator products are normal ordered:

$$:c_{k,\nu,\tau}^{\dagger}c_{k,\nu',\tau'}:=c_{k,\nu,\tau}^{\dagger}c_{k,\nu',\tau'}-\langle c_{k,\nu,\tau}^{\dagger}c_{k,\nu',\tau'}\rangle_{0},$$

where $\nu \in \{R, L\}$. The continuous description is achieved by introducing field operators [14]:

$$c_{k,\nu,\tau}^{\dagger} = \frac{1}{\sqrt{L}} \sum_{n=1}^{L} e^{ik_{\nu}n} c_{n,\nu,\tau}^{\dagger}$$

$$= \sqrt{\frac{D}{L}} \sum_{n=1}^{L} e^{ik_{\nu}D\frac{n}{D}} c_{n,\nu,\tau}^{\dagger} \sqrt{D} \frac{1}{D}$$

$$= \frac{1}{\sqrt{l}} \int_{0}^{l} e^{iq_{k,\nu}x} \psi_{\nu,\tau}^{\dagger}(x) dx ,$$

where x = n/D, $\psi_{\nu,\tau}^{\dagger}(x) = \lim_{D\to\infty} \sqrt{D} c_{n,\nu,\tau}^{\dagger}$, $q_k = k \cdot D$. ψ^{\dagger} , ψ are now fermionic field operators with $\left\{\psi_{\nu,\tau}(x), \psi_{\nu',\tau'}^{\dagger}(x')\right\} = \delta(x-x')\delta_{\nu,\nu'}\delta_{\tau,\tau'}$. Again normal ordering is imposed,

$$: \psi_{\nu,\tau}^{\dagger}(x)\psi_{\nu',\tau'}(x) := \lim_{\epsilon \to 0} \left[\psi_{\nu,\tau}^{\dagger}(x+\epsilon)\psi_{\nu',\tau'}(x) - \langle \psi_{\nu,\tau}^{\dagger}(x+\epsilon)\psi_{\nu',\tau'}(x) \rangle_{0} \right] ,$$

where $\langle \cdots \rangle_0$ is the expectation value in the ground state. Let us summarize the external fields again in an operator H_{ex} . Then

$$\frac{H_h}{2D} = \int_0^l \sum_{\nu,\nu',\tau} \left[\delta_{\nu,\nu'}(\cos k_F + 1) : n_\nu : -\delta_{\nu,\nu'} \mathbb{1}_\nu + i\nu \frac{\sin k_F}{D} : \psi_{\tau,\nu}^{\dagger}(x) \frac{\mathrm{d}}{\mathrm{d}x} \psi_{\tau,\nu'}(x) : \right] \, \mathrm{d}x \;, \quad (31a)$$

$$H_{i} = 2\cos k_{F}J \int_{0}^{l} \delta(x) \sum_{\nu,\nu',\tau} \left[\delta_{\nu,\nu'} n_{d,\tau} \mathcal{P}_{d} : n_{\nu,\tau}(x) : + d_{\tau}^{\dagger} d_{\bar{\tau}} : \psi_{\nu,\bar{\tau}}^{\dagger}(x) \psi_{\nu',\tau}(x) : \right] dx , \qquad (31b)$$

$$H_{ex} = \int_0^l -\mu \left[n(x) + \delta(x) n_d \mathcal{P}_d \right] + \frac{h}{2} \left[\delta(x) (n_{d,\uparrow} - n_{d,\downarrow}) + (n_{\uparrow}(x) - n_{\downarrow}(x)) \right] dx . \tag{31c}$$

The occupation number operators are $n_{\tau,\nu} = :\psi_{\tau,\nu}^{\dagger}\psi_{\tau,\nu}:, n_{\nu} = \sum_{\tau} n_{\tau,\nu}, n_{\tau} = \sum_{\nu} n_{\tau,\nu}.$

As far as the terms (31a), (31b) are concerned, one may pass to a Weyl basis by the canonical transformation

$$\phi_{\pm,\tau}(x) = \frac{1}{\sqrt{2}} \left[\psi_{L,\tau}(x) \pm \psi_{R,\tau}(-x) \right] , \qquad \left\{ \phi_{\nu,\tau}(x), \phi_{\nu',\tau'}^{\dagger}(x') \right\} = \delta(x - x') \delta_{\nu,\nu'} \delta_{\tau,\tau'} .$$

Interaction terms in the host are non-local in the $\phi_{\pm}(x)$; however, as will be shown in the next section these are accounted for by a redefinition of the Fermi velocity v_F , $\sin k_F = v_F \to \tilde{v}_F = v_F (1 + \mathcal{O}(1/\alpha))$. The Weyl basis demonstrates that the impurity couples only with one of the two host channels. The Hamiltonian density thus reads:

$$\mathcal{H}_{h} = 2 \sum_{\tau,\nu=\pm} \left[i\tilde{v}_{F} : \phi_{\nu,\tau}^{\dagger}(x) \frac{\mathrm{d}}{\mathrm{d}x} \phi_{\nu,\tau}(x) : + D(\cos k_{F} + 1) : n_{\nu}(x) : - D \mathbb{1}_{\nu} \right]$$
(32)

$$\mathcal{H}_i = 4J\cos k_F \sum_{\tau} \delta(x) \left[:\phi^{\dagger}_{+,\tau}(x)\phi_{+,\tau}(x) : n_{d,\tau}\mathcal{P}_d + :\phi^{\dagger}_{+,\tau}(x)\phi_{+,\bar{\tau}}(x) : d^{\dagger}_{\bar{\tau}}d_{\tau} \right]$$

$$\mathcal{H}_{ex} = -\mu \left[n(x) + \delta(x) n_d \right] + \frac{h}{2} \left[\delta(x) (n_{d,\uparrow} - n_{d,\downarrow}) + n_{\uparrow}(x) - n_{\downarrow}(x) \right] .$$

The fermionic operators of the impurity can be expressed in terms of spin operators with index i,

$$\sigma_i^z = n_{d,\uparrow} - n_{d,\downarrow}, \ \sigma_i^+ = d_{\uparrow}^{\dagger} d_{\downarrow}, \ \sigma_i^- = d_{\downarrow}^{\dagger} d_{\uparrow}.$$

Then one directly recognizes that the impurity operator is su(2)-symmetric and can be completed to the XXX-exchange operator,

$$\mathcal{H}_{i} = 2J\delta(x)\sum_{\tau,\tau'}:\phi_{+,\tau}^{\dagger}(x)\boldsymbol{\sigma}_{\tau,\tau'}\phi_{+,\tau'}(x):\boldsymbol{\sigma}_{i} + 2J\delta(x)n_{d}\mathcal{P}_{d}:n_{+}(x):, \qquad (33)$$

where $\sigma = (\sigma^x, \sigma^y, \sigma^z)^T$ and $2\cos k_F J_\alpha =: J$ is defined. Eq. (33) constitutes the isotropic Kondo model.

3. Calculation of the free energy

Taking account of eq. (18),

$$e^{-\beta H_h} = \lim_{N \to \infty} \left[\bar{\tau}_h(u_N) \, \tau_h(u_N) \right]^{N/2}, \ u_N = -\frac{\beta D(\alpha + 1)}{N}$$

$$e^{-\beta H} = \lim_{N \to \infty} \left[\bar{\tau}(u_N) \, \tau(u_N) \right]^{N/2} e^{-\beta H_{ex}}$$

$$e^{-\beta H_{ex}} = \prod_{j=1}^{L} e^{-\beta [h/2(n_{j,\uparrow} - n_{j,\downarrow}) - \mu n_j]} e^{-\beta [h/2(n_{d,\uparrow} - n_{d,\downarrow}) - \mu \sum_{\tau} n_{d,\tau}]} =: e^{-\beta \sum_{j=1}^{L} h_{ex,j}} e^{-\beta H_{ex,i}}.$$

The even integer N is referred to as Trotter number and is the height of the fictitious underlying square lattice, see fig. (1). The impurity contribution to the free energy is

$$f_i = -\lim_{L \to \infty} \lim_{N \to \infty} \frac{1}{\beta} \left\{ \ln \operatorname{tr} \left[\left[\bar{\tau}(u_N) \, \tau(u_N) \right]^{N/2} e^{-\beta H_{ex}} \right] - \ln \operatorname{tr} \left[\left[\bar{\tau}_h(u_N) \, \tau_h(u_N) \right]^{N/2} e^{-\beta H_{ex,h}} \right] \right\},$$

where $H_{ex,h} = \sum_{j=1}^{L} h_{ex,j}$. The crucial idea in calculating f_i is to exchange tr and str in the expression

$$\operatorname{tr}\left\{\left[\overline{\tau}(u_{N})\,\tau(u_{N})\right]^{N/2} e^{-\beta H_{ex}}\right\} = \operatorname{tr} e^{-\beta H_{ex}} \prod_{k=1}^{N/2} \operatorname{str}_{a_{2k}a_{2k-1}} \left[\overline{R}_{a_{2k}L}^{(4,4)}(-u_{N}) \dots \overline{R}_{a_{2k}1}^{(4,4)}(-u_{N})\right] \times \overline{R}_{a_{2k}0}^{(4,3)}(-u_{N} + \mathrm{i}u_{0}) R_{a_{2k-1}L}^{(4,4)}(u_{N}) \dots R_{a_{2k-1}1}^{(4,4)}(u_{N}) R_{a_{2k-1}1}^{(4,3)}(u_{N} + \mathrm{i}u_{0})\right].$$

This leads to

$$\operatorname{str} \prod_{j=1}^{L} \left[\operatorname{tr}_{j} e^{-\beta h_{ex,j}} \prod_{k=1}^{N/2} \overline{R}_{a_{2k}j}^{(4,4)}(-u_{N}) R_{a_{2k-1}j}^{(4,4)}(u_{N}) \right] \\
\times \left[\operatorname{tr}_{0} e^{-\beta H_{ex,i}} \prod_{k=1}^{N/2} \overline{R}_{a_{2k}0}^{(4,3)}(-u_{N} + \mathrm{i}u_{0}) R_{a_{2k-1}0}^{(4,3)}(u_{N} + \mathrm{i}u_{0}) \right] =: \operatorname{str} \left[\tau_{h}^{(Q)}(0) \right]^{L} \tau_{i}^{(Q)}(u_{0})$$

$$\tau_h^{(Q)}(v) := \operatorname{tr}_j e^{-\beta h_{ex,j}} \prod_{k=1}^{N/2} \overline{R}_{a_{2k}j}^{(4,4)}(-u_N + iv) R_{a_{2k-1}j}^{(4,4)}(u_N + iv) =: \operatorname{tr}_j T_h^{(Q)}(v)$$
(34)

$$\tau_i^{(Q)}(v) := \operatorname{tr}_0 e^{-\beta H_{ex,i}} \prod_{k=1}^{N/2} \overline{R}_{0,a_{2k}}^{(3,4)}(-u_N + \mathrm{i}v) R_{0,a_{2k-1}j}^{(3,4)}(u_N + \mathrm{i}v) =: \operatorname{tr}_0 T_i^{(Q)}(v) . \tag{35}$$

Eqs. (34), (35) define the Quantum Transfer Matrix (QTM) $\tau_h^{(Q)}$ of the host and $\tau_i^{(Q)}$ of the impurity, respectively. Note that the host matrix is independent of the lattice site j. Each QTM is the trace over the auxiliary space of a Quantum Monodromy Matrix $T^{(Q)}$. The auxiliary space of $\tau_h^{(Q)}$ is four-dimensional, of $\tau_i^{(Q)}$ three-dimensional. Fig. 1 depicts this "rotation" from auxiliary space into quantum space. Due to eqs. (3), (10),

$$\left[\tau_{\nu}^{(Q)}(v), \tau_{\nu'}^{(Q)}(v')\right] = 0, \tag{36}$$

where the symbolical indices ν, ν' may take values h, i. The auxiliary spectral parameter is essential for the diagonalization of $\tau^{(Q)}$, the u_N are inhomogeneities with alternating signs. Especially, eq. (36) holds for $\nu \neq \nu'$: The impurity and host QTM's share the same set of eigenvectors. The largest eigenvalue of $\tau^{(Q)}_{\nu}$ is separated by a gap from the rest of the spectrum for any N. The eigenstate $|\Phi_{\max}\rangle$ leading to the largest eigenvalue $\Lambda^{\max}_i(v)$ of $\tau^{(Q)}_i(v)$ also leads to the largest eigenvalue $\Lambda^{\max}_h(v)$ of $\tau^{(Q)}_h(v)$. Although interesting, this is not essential: The dominant eigenstate $|\Phi_{\max}\rangle$ of the host matrix $\tau^{(Q)}_h(v)$ determines the "correct" eigenvalue of the impurity matrix $\tau^{(Q)}_i$:

$$\ln \left[\operatorname{str} \left(\tau_h^{(Q)}(0) \right)^L \tau_0^{(Q)}(u_0) \right]$$

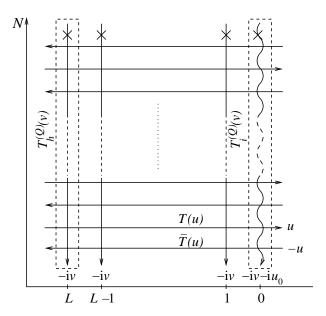


Figure 1. Classical lattice representing the free energy of the impurity model. L is the physical, N the Trotter direction. The dimension in the impurity quantum space (wavy line) is reduced by one. The spectral parameter on the straight vertical lines is 0 and on the wavy vertical line $-iu_0$. For the further analysis it is convenient to introduce the auxiliary spectral parameter -iv on the vertical lines. Crosses stand for twisted boundary conditions, induced by external fields h and μ .

$$= \ln \left[(-1)^{p[\max]} \left(\Lambda_h^{\max}(0) \right)^L \Lambda_i^{\max}(u_0) + \sum_{k \neq \max} (-1)^{p[k]} \left(\Lambda_h^{(k)}(0) \right)^L \Lambda_i^{(k)}(u_0) \right]$$
(37a)

$$\sim \ln\left[(\Lambda_h^{\max}(0))^L \Lambda_i^{\max}(u_0) \right] + \sum_{k \neq \max} (-1)^{p[k]} \left(\frac{\Lambda_h^{(k)}(0)}{\Lambda_h^{\max}(0)} \right)^L \frac{\Lambda_i^{(k)}(u_0)}{\Lambda_i^{\max}(u_0)} , \tag{37b}$$

which is an asymptotical expansion for large L. Generally, the eigenstate of the kth largest eigenvalue of $\tau_h^{(Q)}$ does not lead to the kth largest eigenvalue of $\tau_i^{(Q)}$. So with respect to $\tau_i^{(Q)}$, k does not label the eigenvalues according to their order. The supertrace requires to include the parity of the projector on the eigenstate k. Note that $p[\max] = 0$. In [19] it is argued that the two limits $N \to \infty$, $L \to \infty$ are interchangeable. Then the thermodynamic limit $L \to \infty$ in eq. (37b) is carried out just by keeping the largest eigenvalues $\Lambda_{h,I}^{\max}$.

One concludes that the impurity and host contribution to the free energy per lattice site are given by

$$f_i = -\lim_{N \to \infty} \frac{1}{\beta} \ln \Lambda_i^{\text{max}}(u_0)$$
 (38)

$$f_h = -\lim_{N \to \infty} \frac{1}{\beta} \ln \Lambda_h^{\text{max}}(0)$$
(39)

Eqs. (38), (39) summarize the enormous advantage of considering the QTM: The calculation of the free energy is reduced to the evaluation of a single eigenvalue.

 f_h has already been calculated in this approach [20, 21], the result is given below. The diagonalization of $\tau_h^{(Q)}$ is done by applying techniques of the nested Algebraic Bethe Ansatz (NABA) [15], yielding for the eigenvalue Λ_i of the non-normalized QTM $\tau_i^{(Q)}$:

$$\Lambda_{i}(v) = \lambda_{-}(v) + \lambda_{+}(v) + \lambda_{0}(v)$$

$$\lambda_{-}(v) = \frac{q_{-}(v+i)}{q_{-}(v)} \phi_{+}(v+i\alpha/2) \phi_{-}(v-i\alpha/2-i) e^{\beta(\mu+h/2)}$$

$$\lambda_{+}(v) = \frac{q_{+}(v-i)}{q_{+}(v)} \phi_{-}(v-i\alpha/2) \phi_{+}(v+i\alpha/2+i) e^{\beta(\mu-h/2)}$$

$$\lambda_{0}(v) = \frac{q_{-}(v+i)q_{+}(v-i)}{q_{-}(v)q_{+}(v)} \phi_{+}(v-i\alpha/2) \phi_{-}(v+i\alpha/2)$$

$$q_{+}(v) = \prod_{i=1}^{M} (v-v_{i}), q_{-}(v) = \prod_{k=1}^{\widetilde{M}} (v-\tilde{v}_{k}), \phi_{\pm}(v) = (v\pm iu)^{N/2}.$$
(40)

An external magnetic field h and a chemical potential μ have been introduced. The roots - or particle solutions - $\{v_i\}$, $\{\tilde{v}_k\}$ are determined by the analyticity of the eigenvalue:

$$\frac{\lambda_{+}(v_{j})}{\lambda_{0}(v_{j})} = \left. \frac{q_{-}(v)}{q_{-}(v+i)} \frac{\phi_{-}(v-i\alpha/2) \phi_{+}(v+i+i\alpha/2)}{\phi_{+}(v-i\alpha/2) \phi_{-}(v+i\alpha/2)} e^{\beta(\mu-h/2)} \right|_{v=v_{j}} = -1$$
(41a)

$$\frac{\lambda_{-}(\tilde{v}_{k})}{\lambda_{0}(\tilde{v}_{k})} = \left. \frac{q_{+}(v)}{q_{+}(v-i)} \frac{\phi_{+}(v+i\alpha/2) \phi_{-}(v-i-i\alpha/2)}{\phi_{+}(v-i\alpha/2) \phi_{-}(v+i\alpha/2)} e^{\beta(\mu+h/2)} \right|_{v=\tilde{v}_{k}} = -1.$$
(41b)

These Bethe-Ansatz equations are $M+\widetilde{M}$ many nonlinear coupled algebraic equations for the unknown roots. Using analyticity properties, we represent the eigenvalue by a finite set of non-linear integral equations (NLIE). Within this approach, the Trotter limit $N\to\infty$ is carried out analytically. Consider the following combinations of $\lambda_{\pm,0}$, eq. (40):

$$\frac{1}{\mathfrak{b}(v)} := \frac{\lambda_{+}(v)}{\lambda_{-}(v)} \left(1 + \frac{\lambda_{0}(v)}{\lambda_{+}(v)} \right) \\
= \frac{q_{+}(v-i)}{q_{-}(v+i)} \frac{\phi_{-}(v-i\alpha/2) \phi_{+}(v+i+i\alpha/2)}{\phi_{+}(v+i\alpha/2) \phi_{-}(v-i-i\alpha/2)} e^{-\beta h} \\
\times \underbrace{\frac{q_{-}(v)}{q_{+}(v)} \left(1 + \frac{q_{-}(v+i)}{q_{-}(v)} \frac{\phi_{+}(v-i\alpha/2) \phi_{-}(v+i\alpha/2)}{\phi_{-}(v-i\alpha/2) \phi_{+}(v+i+i\alpha/2)} e^{-\beta(\mu-h/2)} \right)}_{\equiv \frac{q_{-}^{(h)}(v)}{\phi_{-}(v-i\alpha/2) \phi_{+}(v+i+i\alpha/2)}} \\
= \frac{1}{\phi_{+}(v+i\alpha/2)\phi_{-}(v-i-i\alpha/2)} \frac{q_{+}(v-i)}{q_{-}(v+i)} q_{-}^{(h)}(v) e^{-\beta h}, \tag{42}$$

where $q_-^{(h)} := \prod_{j=1}^{N-M+\widetilde{M}} \left(v - \widetilde{v}_j^{(h)}\right)$, and $\widetilde{v}_j^{(h)}$ are called hole solutions. The polynomial $q_-^{(h)}$ has been identified by reasons of analyticity: The zeroes of numerator and denominator cancel as far as the particle solutions are concerned, the hole solutions rest as zeroes of the numerator. The polynomials in the denominator are the same

as the ϕ -terms in λ_0/λ_+ . Along the same reasoning (or simply by taking the complex conjugate and $h \to -h$), we find another function $\overline{\mathfrak{b}}$:

$$\frac{1}{\overline{\mathfrak{b}}(v)} := \frac{\lambda_{-}(v)}{\lambda_{+}(v)} \left(1 + \frac{\lambda_{0}(v)}{\lambda_{-}(v)} \right)
= \frac{1}{\phi_{-}(v - i\alpha/2)\phi_{+}(v + i + i\alpha/2)} \frac{q_{-}(v + i)}{q_{+}(v - i)} q_{+}^{(h)}(v) e^{\beta h} ,$$
(43)

where $q_{+}^{(h)} := \prod_{j=1}^{N-\widetilde{M}+M} \left(v-v_{j}^{(h)}\right)$. A third function \mathfrak{c} is introduced,

$$\frac{1}{\mathfrak{c}(v)} := \frac{\lambda_0(v)}{\lambda_+(v) \, \lambda_-(v)} \, \Lambda_i(v)
= \frac{\phi_+(v - i\alpha/2) \, \phi_-(v + i\alpha/2) \, \mathrm{e}^{-2\beta\mu}}{\phi_-(v - i\alpha/2) \, \phi_+(v + i + i\alpha/2) \, \phi_+(v + i\alpha/2) \, \phi_-(v - i\alpha/2 - i)} \, \Lambda_i(v) \, . \quad (44)$$

Consider $\mathfrak{B} := 1 + \mathfrak{b}, \ \overline{\mathfrak{B}} := 1 + \overline{\mathfrak{b}}, \ \mathfrak{C} := 1 + \mathfrak{c},$

$$\begin{split} \mathfrak{B}(v) &= \frac{1}{\lambda_{-}(v)} \, \mathfrak{b}(v) \, \Lambda_{i}(v) = \frac{q_{-}(v)}{q_{+}(v-\mathrm{i}) \, q_{-}^{(h)}(v)} \, \Lambda_{i}(v) \, \mathrm{e}^{-\beta(\mu-h/2)} \\ \overline{\mathfrak{B}}(v) &= \frac{1}{\lambda_{+}(v)} \, \overline{\mathfrak{b}}(v) \, \Lambda_{i}(v) = \frac{q_{+}(v)}{q_{-}(v+\mathrm{i}) \, q_{+}^{(h)}(v)} \, \Lambda_{i}(v) \, \mathrm{e}^{-\beta(\mu+h/2)} \\ \mathfrak{C}(v) &= \frac{1}{\mathfrak{b}(v) \, \overline{\mathfrak{b}}(v)} \, \mathfrak{c}(v) = \frac{q_{+}^{(h)}(v) \, q_{-}^{(h)}(v)}{\phi_{+}(v-\mathrm{i}\alpha/2) \, \phi_{-}(v+\mathrm{i}\alpha/2)} \, \frac{1}{\Lambda_{i}(v)} \, \mathrm{e}^{2\beta\mu} \; . \end{split}$$

In Appendix B, the unknown functions $q_{\pm}, q_{\pm}^{(h)}, \Lambda_i$ are expressed through the auxiliary functions by means of analyticity arguments for the largest eigenvalue. The result is a closed set of NLIE:

$$\ln \mathfrak{b}(v) = \phi_{\mathfrak{b}}(v + \mathrm{i}\delta) - [k_{\mathfrak{b}} * \ln \overline{\mathfrak{B}}](v + 2\mathrm{i}\delta) - [k_{\mathfrak{b}} * \ln \mathfrak{C}](v + \mathrm{i}\delta) + \beta(\mu + h/2) \tag{45a}$$

$$\ln \overline{\mathfrak{b}}(v) = \phi_{\overline{\mathfrak{b}}}(v - \mathrm{i}\delta) - [k_{\overline{\mathfrak{b}}} * \ln \mathfrak{B}](v - 2\mathrm{i}\delta) - [k_{\overline{\mathfrak{b}}} * \ln \mathfrak{C}](v - \mathrm{i}\delta) + \beta(\mu - h/2) \tag{45b}$$

$$\ln \mathfrak{c}(v) = \phi_{\mathfrak{c}}(v) - [k_{\mathfrak{b}} * \ln \overline{\mathfrak{B}}](v + i\delta) - [k_{\overline{\mathfrak{b}}} * \ln \mathfrak{B}](v - i\delta) - [k_{\mathfrak{c}} * \ln \mathfrak{C}](v) + 2\beta\mu \tag{45c}$$

The contributions of the impurity and host to the free energy are given by:

$$-\beta f_i = -\ln \mathfrak{c}(u_0) - 2\beta D(\alpha + 1)J_\alpha + 2\beta \mu \tag{46}$$

$$-\beta f_h = \eta(0) + [\zeta * \ln \mathfrak{B}](0) + [\overline{\zeta} * \ln \overline{\mathfrak{B}}](0) + [(\zeta + \overline{\zeta}) * \ln \mathfrak{C}](0)$$
 (47)

The inhomogeneities are

$$\phi_{\mathfrak{b}}(v) = -\frac{\beta D(\alpha+1)^2}{(v+\mathrm{i}\alpha/2)(v-\mathrm{i}\alpha/2-\mathrm{i})}, \ \phi_{\overline{\mathfrak{b}}} = \phi_{\mathfrak{b}}^*$$

$$\tag{48}$$

$$\phi_{\mathfrak{c}} = \phi_{\mathfrak{b}} + \phi_{\overline{\mathfrak{b}}} \,. \tag{49}$$

The convolutions $[f * g](x) := \int_{-\infty}^{\infty} f(x - y)g(y)dy$ involve local kernels:

$$k_{\mathfrak{b}}(v) = \frac{1}{2\pi v(v-\mathrm{i})}, \ k_{\overline{\mathfrak{b}}} = k_{\mathfrak{b}}^*, \ k_{\mathfrak{c}} = k_{\mathfrak{b}} + k_{\overline{\mathfrak{b}}}$$
$$2\pi \zeta(v) = -\frac{\phi_{\mathfrak{b}}(-v)}{D\beta(\alpha+1)}, \ \eta(v) = 2\beta D \frac{(\alpha+1)^2}{v^2 + (\alpha+1)^2}$$

Following the treatment of the Hamiltonian in the preceding section, we want to perform an asymptotic expansion of the free energy in the limit $\alpha \gg 1$. The essential observation from the study of the Hamiltonian is that after the canonical transformation, excitations of the impurity stem exclusively from transitions between singly occupied states. Furthermore, it was argued that u_0 has to be scaled such that zero occupation is energetically suppressed. First consider the case where u_0 is held fixed. By scaling $v \to \alpha v$, the algebraically decaying kernels shrink to δ -functions. The leading contribution thus solely stems from the driving terms $\phi_{\mathfrak{b},\overline{\mathfrak{b}},\mathfrak{c}}$. Within this approximation, the auxiliary functions can be calculated explicitly:

$$\mathfrak{b}(\alpha v) = \frac{a(\alpha v)}{1 + \overline{a}(\alpha v)}, \ \overline{\mathfrak{b}}(\alpha v) = \frac{\overline{a}(\alpha v)}{1 + a(\alpha v)}, \ \mathfrak{c}(\alpha v) = \frac{a(\alpha v)\overline{a}(\alpha v)}{1 + a(\alpha v) + \overline{a}(\alpha v)}$$

$$a(v) = \exp\left[\phi_{\mathfrak{b}}(v + i/2) + \beta(\mu + h/2)\right], \ \overline{a}(v) = \exp\left[\phi_{\overline{\mathfrak{b}}}(v - i/2) + \beta(\mu - h/2)\right].$$
(50)

The quantity δ in eqs. (45a)-(45c) has been chosen $\delta = 1/2$ such that a, \overline{a} are real valued functions. Define $\lim_{\alpha \to \infty} (\alpha + 1) J_{\alpha} =: J_0$. From the expression of f_i , eq. (46) it then follows that the free energy is that of an uncoupled impurity,

$$\lim_{\alpha \to \infty} f_i(T, h) = -T \ln \left[(a\overline{a})^{-1}(u_0) + a^{-1}(u_0) + \overline{a}^{-1}(u_0) \right] + 2DJ_0 - 2\mu$$

$$= -T \ln \left[e^{\beta 2DJ_0} + e^{\beta(\mu + h/2)} + e^{\beta(\mu - h/2)} \right] . \tag{51}$$

The free energy reflects the expected result of a free impurity with three possible states, namely empty and singly occupied with up or down spin. A more detailed analysis of the case where u_0 is held fixed will be given in a forthcoming publication [10]. We now demonstrate that the two latter states dominate if u_0 is scaled appropriately with α, D, μ , such that a crossover temperature emerges, below which a strong coupling fixed point is reached.

For low temperatures, the auxiliary function \mathfrak{c} exhibits a sharp crossover from $\mathfrak{c} \ll 1$ to $\mathfrak{c} \gg 1$ in regions around "Fermi points" $\pm \Lambda_{\mathfrak{c}}$ defined by

$$-\phi_{\rm c}(\Lambda_{\rm c}) \approx 2\beta\mu$$
, $\Lambda_{\rm c} \approx \pm \alpha \sqrt{\frac{D}{\mu} - \frac{1}{4}}$. (52)

Set $h \ll \mu$. The influence of h on the Fermi points is neglected, since it enters quadratically. The more common parameterization is

$$\frac{v}{\alpha} = \frac{1}{2} \tan \frac{k}{2} \,, \tag{53}$$

where k is the wave-vector used in the Fourier representation of the Hamiltonian in the preceding section (not the Fourier variable conjugate to v). At $v = \Lambda_c$, eq. (52) is equivalent to

$$2D(\cos k_F + 1) = \mu , \qquad (54)$$

which defines k_F at constant μ at $D \gg T$, such that $\mu = \epsilon_F$ (μ in turn is related to the particle number N by $k_F = \pi N/(2L)$. Then eq. (54) yields a relation between μ and N, independent of T - this demonstrates that the formally grand-canonical description

is effectively canonical, because $D \gg T$). For the analysis of the NLIE, consider

$$k_{\mathfrak{c},\mathfrak{b}} * \ln \mathfrak{C}(v) = k_{\mathfrak{c},\mathfrak{b}} * \ln \mathfrak{c}(v) + \int_{|w| < \Lambda_{\mathfrak{c}}} k_{\mathfrak{c},\mathfrak{b}}(v - w) \ln \frac{\mathfrak{C}(w)}{\mathfrak{c}(w)} dw . \tag{55}$$

To evaluate the second integrand, note that asymptotically,

$$\frac{\mathfrak{C}}{\mathfrak{c}} = \frac{1}{a\overline{a}}(1+a)(1+\overline{a}) = O\left(\frac{1}{\mathfrak{b}\overline{\mathfrak{b}}}\right) \tag{56}$$

$$\ln \frac{\mathfrak{C}(v)}{\mathfrak{c}(v)} = \begin{cases} \ln\left[\left(1 + a(v)\right)\left(1 + \overline{a}(v)\right)\right] + \left[-\phi_{\mathfrak{c}}(v) - 2\beta\mu\right], & |v| < \Lambda_{\mathfrak{c}} \\ 0, & |v| > \Lambda_{\mathfrak{c}} \end{cases}$$
 (57)

Consider the case $|v| < \Lambda_{\mathfrak{c}}$ in eq. (57). The first term is exponentially small, the second term dominates. It is inserted into the second integrand on the rhs of eq. (55) which shall be considered as a next-leading correction compared to the driving terms in eqs. (45a)-(45c). In view of eq. (46), the most interesting range of the spectral parameter is $v \sim v_0$. Set

$$|u_0| = |v_0/2| > \Lambda_{\mathfrak{c}} \sim \alpha \,, \tag{58}$$

as indicated in (25). Then one proceeds with eq. (55)

$$k_{\mathfrak{c},\mathfrak{b}} * \ln \mathfrak{C}(v) \stackrel{|v| > \Lambda_{\mathfrak{c}}}{\approx} k_{\mathfrak{c},\mathfrak{b}} * \ln \mathfrak{c}(v) + k_{\mathfrak{c},\mathfrak{b}}(v) \int_{|w| < \Lambda_{\mathfrak{c}}} \ln \frac{\mathfrak{C}(w)}{\mathfrak{c}(w)} \mathrm{d}w + \mathrm{O}(1/v^4) \ .$$

As an estimate for the second term on the rhs, one uses the leading term of eq. (57):

$$\ln \frac{\mathfrak{C}(v)}{\mathfrak{c}(v)} = [-\phi_{\mathfrak{c}}(v) - 2\beta\mu] + O(\exp[-\beta D])$$

$$\int_{|w|<\Lambda_{\mathfrak{c}}} \ln \frac{\mathfrak{C}(w)}{\mathfrak{c}(w)} dw \approx 4\beta \alpha D \left[2 \arctan \frac{2\Lambda_{\mathfrak{c}}}{\alpha} - \frac{\mu \Lambda_{\mathfrak{c}}}{\alpha D} + O(1/\alpha) \right] =: \beta \kappa > 0.$$
 (59)

The sub-leading order $O(1/\alpha)$ is neglected in the following, which is justified rigorously below. The above defined quantity κ is a monotonously decreasing function of μ/D . Choose $\Lambda_{\mathfrak{c}} > 0$ such that $\kappa > 0$. Summarizing,

$$k_{\mathfrak{b},\mathfrak{c}} * \ln \mathfrak{C} = k_{\mathfrak{b},\mathfrak{c}} * \ln \mathfrak{c} + \beta \kappa k_{\mathfrak{b},\mathfrak{c}} , \qquad (60)$$

so that $\ln \mathfrak{C}$ can be eliminated in eqs. (45*a*)-(45*c*). The Fourier transforms of $\phi_{\mathfrak{b}}$, $\phi_{\overline{\mathfrak{b}}}$, $\phi_{\mathfrak{c}}$, eqs. (48), (49) are:

$$\hat{\phi}_{\mathfrak{b}}(k) = -\beta D(\alpha + 1) \begin{cases} e^{-\alpha/2k}, & k \ge 0 \\ e^{(\alpha/2+1)k}, & k < 0 \end{cases}$$

$$\hat{\phi}_{\overline{\mathfrak{b}}}(k) = -\beta D(\alpha + 1) \begin{cases} e^{-(\alpha/2+1)k}, & k \ge 0 \\ e^{\alpha/2k}, & k < 0 \end{cases}$$

$$\hat{\phi}_{\mathfrak{c}}(k) = \hat{\phi}_{\mathfrak{b}}(k) + \hat{\phi}_{\overline{\mathfrak{b}}}(k) = -\beta D(\alpha + 1) \begin{cases} e^{-\alpha/2k} \left(1 + e^{-k}\right), & k \ge 0 \\ e^{\alpha/2k} \left(1 + e^{k}\right), & k < 0 \end{cases}$$

$$(61)$$

Inserting eq. (60) gives, using eqs. (45a)-(45c):

$$\hat{\mathfrak{c}}(k) = \begin{cases} \frac{\hat{\phi}_{\mathfrak{c}}}{1 + e^{-k}} - \frac{1}{1 + e^{k}} \beta \kappa - \frac{\hat{\overline{\mathfrak{B}}} + e^{-k} \hat{\mathfrak{B}}}{1 + e^{-k}} & k \ge 0\\ \frac{\hat{\phi}_{\mathfrak{c}}}{1 + e^{k}} - \frac{1}{1 + e^{-k}} \beta \kappa - \frac{\hat{\mathfrak{B}} + e^{k} \hat{\overline{\mathfrak{B}}}}{1 + e^{k}} & k < 0 \end{cases}$$

$$(62a)$$

$$\hat{\mathfrak{b}}(k) = -\frac{1}{1 + e^{-k}} \beta \kappa + \frac{1}{1 + e^{|k|}} (\hat{\mathfrak{B}} - \hat{\overline{\mathfrak{B}}})$$
(62b)

$$\hat{\bar{\mathfrak{b}}}(k) = -\frac{1}{1 + e^k} \beta \kappa + \frac{1}{1 + e^{|k|}} (\hat{\bar{\mathfrak{B}}} - \hat{\mathfrak{B}})$$
(62c)

Note that in the limit $\Lambda_{\mathfrak{c}} \to 0$, i.e. $\mu \to 4D$, the resulting equations are trivially solved; $\ln \mathfrak{b} = \beta h = -\ln \overline{\mathfrak{b}}$, and $\mathfrak{B} = 1 + \exp(\beta h)$, $\overline{\mathfrak{B}} = 1 + \exp(-\beta h)$,

$$f_i = \text{const.} + \ln\left(e^{\beta h/2} + e^{-\beta h/2}\right) ,$$
 (63)

which is the free energy of a free, uncoupled spin. This situation corresponds to a completely filled band.

The NLIE eq. (62a)-(62c) are transformed back to direct space,

$$\ln \mathfrak{b}(v) = -2\pi \beta \kappa \Phi(v + i\delta) + \beta h/2 + [k * \ln \mathfrak{B}](v) - [k * \ln \overline{\mathfrak{B}}](v + 2i\delta)$$
(64a)

$$\ln \overline{\mathfrak{b}}(v) = 2\pi \beta \kappa \Phi(v - i\delta) - \beta h/2 + [k * \ln \overline{\mathfrak{B}}](v) - [k * \ln \mathfrak{B}](v - 2i\delta)$$
(64b)

$$\ln \mathfrak{c}(v) = -\beta D(\alpha + 1) \frac{\alpha}{v^2 + \alpha^2/4} - k(v)\beta \kappa + \beta \mu$$

$$+ \left[\Phi * \ln \mathfrak{B}\right](v - \mathrm{i}\delta) - \left[\Phi * \ln \overline{\mathfrak{B}}\right](v + \mathrm{i}\delta) . \tag{64c}$$

The driving term and integration kernel read:

$$\Phi(v) = \frac{1}{2\sinh \pi v}$$

$$k(v) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-|k|/2}}{2\cosh k/2} e^{ikv} dk.$$

Choose $\delta=1/2$ and scale v by $1/\pi$. Since Φ decays exponentially, it is possible to absorb κ and v_0 in a new additive constant. Substitute

$$v = x - \ln(2\pi\kappa) \tag{65}$$

and remember that κ scales with αD (59) and therefore may be arbitrarily large. All parameters can be combined in the free energy to a new constant T_K ,

$$-\ln(2\pi\kappa) - \pi v_0/2 =: -\ln T_K , \qquad T_K = 2\pi\kappa e^{\pi v_0/2} . \tag{66}$$

The range of $|v_0|$ has been identified in eq. (58), we take $v_0 = -|v_0|$. The shift (65) scales the driving term $\Phi(v/\pi - i/2)$:

$$-2\beta\pi\kappa\Phi(v/\pi - i/2) = -\frac{\beta\pi\kappa}{\cosh v}$$

$$= -\frac{2\beta\pi\kappa}{e^{x-\ln(2\pi\kappa)} + e^{-x+\ln(2\pi\kappa)}}$$

$$\stackrel{\kappa \to \infty}{=} -\beta e^{x}.$$
(67)

In the second line, eq. (65) has been employed. At this point it is clear that sub-leading orders in eq. (59) can safely be neglected. Furthermore, a factor β can be absorbed by shifting $x \to x - \ln \beta$:

$$\ln \mathfrak{b}(x) = -e^x + \beta h/2 + [k * \ln \mathfrak{B}](x) - [k * \ln \overline{\mathfrak{B}}](x + i\pi - i\epsilon) \tag{68a}$$

$$\ln \overline{\mathfrak{b}}(x) = -e^x - \beta h/2 + [k * \ln \overline{\mathfrak{B}}](x) - [k * \ln \mathfrak{B}](x - i\pi + i\epsilon)$$
 (68b)

$$-\beta f_i = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\left[\ln \mathfrak{B}\overline{\mathfrak{B}}\right](x)}{\cosh\left(x + \ln \frac{T}{T_K}\right)} dx.$$
 (68c)

As far as the host is concerned, equations (50) are inserted into equation (47):

$$-\lim_{\alpha\to\infty}\beta f_h = \eta(0) + \frac{1}{2\pi} \int_{\Lambda_c/\alpha}^{\Lambda_c/\alpha} \frac{1}{v^2 + 1/4} \ln\left[(1 + a(v))(1 + \overline{a}(v)) \right] dv.$$

Observe the relation between the elementary excitation energy $\epsilon(v)$ and the momentum k(v) as functions of the spectral parameter v (cf. eq. (53)),

$$\epsilon(v) = \frac{\mathrm{d}}{\mathrm{d}v}k(v) \ . \tag{69}$$

Then one obtains the energy-momentum relation $\epsilon(k)$:

$$\epsilon(v) = \frac{1}{v^2 + 1/4} \rightarrow k(v) = 2 \arctan 2v$$

$$\epsilon(k) = 4 \cos^2 \frac{k}{2} = 2 \cos k + 2 \tag{70}$$

The function k(v) in the first line is given by eq. (69). From eqs. (59), (66), D gets arbitrarily large, leading to a linear dispersion in the host. Then the free energy density f_h of the host is given by:

$$f_h = -\lim_{\beta \gg 1} \frac{T}{2\pi} \int_{-k_F D}^{k_F D} \ln\left[1 + e^{-\beta(\tilde{v}_F|q| - h/2 - \tilde{\mu})}\right] \left[1 + e^{-\beta(\tilde{v}_F|q| + h/2 - \tilde{\mu})}\right] dq$$

$$\tilde{\mu} := \mu - 2D\left(\left(1 + \frac{3}{\alpha}\right)(\cos k_F + 1) - \frac{2}{\alpha}(\cos k_F + 1)^2\right)$$

$$\tilde{v}_F := 2\left(1 + \frac{3}{\alpha} - \frac{4}{\alpha}(\cos k_F + 1)\right)\sin k_F$$

$$,$$

$$(71)$$

where $q = k \cdot D$. Note that interactions in the host of order $O(1/\alpha)$ can be absorbed into a redefinition of $v_F = 2 \sin k_F$, resulting in effectively free fermions. The leading orders of the specific heat and magnetic susceptibility are

$$C_h(T) = T \frac{\pi^2}{3} \frac{2}{\pi \widetilde{v}_F} =: T \frac{\pi^2}{3} \widetilde{\rho}_h \tag{72}$$

$$\chi_h(T) = \frac{1}{4} \frac{2}{\pi \widetilde{v}_F} =: \frac{1}{4} \widetilde{\rho}_h , \qquad (73)$$

where $\widetilde{\rho}_h$ is the density of states in the host.†

4. Calculation of high- and low-temperature scales

We demonstrate the advantage of our novel approach by a direct calculation of highand low-temperature scales and comparison with Wilson's results [4].

Wilson found for $h, T \ll T_K$, the ratio of the specific heat C_i to the magnetic susceptibility χ_i is universal:

$$\chi_i(T) = \frac{1}{2\pi T_K}, \quad C_i(T) = \frac{\pi T}{3T_K}$$

$$R_w := \frac{\chi_i(T)}{C_i(T)} \frac{C_h(T)}{\chi_h(T)} = 2.$$
(74)

† The host in our model, eq. (32), contains two channels. Therefore $\tilde{\rho}_h$ is enhanced by a factor 2. The impurity couples only to one of the two channels.

We confirm these results in our approach by using dilogarithmic identities [22] to extract the lowest order of the free energy for low fields and temperatures,

$$\lim_{T,h \ll T_K} f(T,h) = -\frac{T^2}{2T_K} \frac{\pi}{3} - \frac{1}{4\pi} \frac{h^2}{T_K} \,. \tag{75}$$

From eq. (75),

$$\lim_{T,h \ll T_K} C(T) = \frac{T}{T_K} \frac{\pi}{3} \qquad \lim_{T,h \ll T_K} \chi(h) = \frac{1}{T_K} \frac{1}{2\pi} . \tag{76}$$

This Fermi liquid behavior is to be compared with the host, eqs. (72), (73). Define the coefficient of the linear T-dependence of C_h by δ_h . Then R_w is calculated as

$$R_w := \lim_{T \to 0} \frac{\chi}{\chi_h} \frac{\delta_h}{\delta} = 2. \tag{77}$$

For high T and h = 0, the impurity susceptibility asymptotically reaches the Curie-Weiss limit:

$$\chi(T) = \frac{1}{4T} \left[1 - \frac{1}{x} - \frac{\ln x}{2x^2} + O(x^{-3}) \right]_{x = \ln T/\tilde{T}_K}.$$

 \widetilde{T}_K is defined such that contributions $O\left(\ln^{-2}T/\widetilde{T}_K\right)$ do not occur,

$$\widetilde{T}_K = 2\pi \xi T_K , \qquad \xi = 0.1032 \pm 0.0005 ,$$
 (78)

where the numerical value of ξ was calculated by Wilson [4]. The calculation of the numbers R_w , ξ are benchmarks for any non-perturbative solution of the Kondo model covering the entire temperature axis. In [6], a perturbative expansion of the free energy by Andrei gave an analytical expression of ξ , $\xi = 0.102676...$ This number has not been obtained in the framework of the exact TBA solution yet. However, by analyzing the NLIE eqs. (68a)-(68c) we are now able to give an accurate numerical value of ξ , which is summarized in the rest of this section.

In the high-temperature regime $T \gg T_K$, the asymptotic behavior of the auxiliary functions for $x \sim -\ln T/T_K \ll 0$ gives the main contribution according to eq. (68c). The convolutions in eq. (68a) are evaluated asymptotically at h=0:

Re
$$\ln \mathfrak{B}(x \ll 0) = \ln 2 + \frac{\pi^2}{4 x^3}$$

Re $\partial_{\beta h} \ln \mathfrak{B}(x \ll 0) = \frac{1}{2} + \frac{1}{4 x} - \frac{\ln |x|}{8x^2} + \frac{\phi}{x^2}$ (79)
Re $\partial_{\beta h}^2 \ln \mathfrak{B}(x \ll 0) = \frac{1}{4} \left(1 + \frac{1}{x} - \frac{\ln |x|}{2x^2} + \frac{4\phi + \frac{1}{4}}{x^2} \right)$.

The coefficient ϕ of the x^{-2} -decay in eq. (79) is determined numerically; we find $\phi = 0.04707 \pm 2 \cdot 10^{-7}$. From this one gets $\xi = \exp\left[-4\phi - 1/4\right]/2\pi = 0.102678 \pm 2 \cdot 10^{-6}$, agreeing nicely both with Wilson's and Andrei's results. Details of the calculations will be published in a forthcoming paper [10].

5. Conclusion and outlook

An Anderson-like impurity Hamiltonian on a one-dimensional lattice has been obtained as the logarithmic derivative of a gl(2|1) symmetric transfer matrix. The free energy for the lattice model was calculated exactly from a closed set of finitely many NLIE. As a special case, this impurity model allows for the Kondo limit of a localized magnetic impurity in an interacting host of electrons including the free fermion case. Mathematically, the Kondo limit constitutes the reduction of gl(2|1) symmetry to su(2) symmetry on the impurity site.

We expect that the lattice regularization presented in this work can be generalized to the Kondo model with anisotropic exchange by using the quantum super-algebra $U_q gl(2|1)$. Furthermore, it is possible [25] to find representations of gl(2|1) such that one of its subalgebras is the (2S+1)-dimensional irrep of su(2). This allows for a lattice path integral approach to multichannel spin-S Anderson-like models. In a forthcoming paper [10], we will give the corresponding closed set of NLIE in the Kondo limit. These can be obtained by an argument of symmetry, and allow for the calculation of Wilson ratios in the general multichannel spin-S case. After having found a lattice path integral approach in the simplest case (spin-1/2, single channel), the next question addresses two-point correlation functions like $\langle \sigma_i^{\mu} \sigma_r^{\mu'} \rangle$, $r = 1, \ldots, L$. Since the spectrum and the corresponding eigenstates of $T_{h,i}^{(Q)}$ are known, those quantities can be calculated in principle, by generalizing methods developed in [26] to graded models. In view of progress in describing the screening cloud around the impurity at $T \ll T_K$ by methods of conformal field theory [23, 24] complementary understanding from the exact solution is highly desirable. Finally, the Anderson impurity model on the lattice, including charge fluctuations, can be treated exactly by solving eqs. (45a)-(45c), a question currently under investigation.

We acknowledge very useful discussions with F. Göhmann.

Appendix A. Alternative fermionization and gl(2|1)-symmetry

Appendix A.1. Alternative fermionization

The matrices X and Y defined in (14), (15) provide one possible fermionic representation of the $[m_j]_a^b$, $[e_0]_a^b$. This representation is not unique: In this appendix, we use slightly modified matrices \widetilde{X} , \widetilde{Y} . However, the fermionic representation of the Hamiltonian is essentially the same. Consider

$$\widetilde{X}_{j} = \begin{pmatrix} (1 - n_{j\downarrow})(1 - n_{j\uparrow}) & (1 - n_{j\downarrow})c_{j\uparrow} & c_{j\downarrow}(1 - n_{j\uparrow}) & c_{j\downarrow}c_{j\uparrow} \\ (1 - n_{j\downarrow})c_{j\uparrow}^{\dagger} & (1 - n_{j\downarrow})n_{j\uparrow} & -c_{j\downarrow}c_{j\uparrow}^{\dagger} & -c_{j\downarrow}n_{j\uparrow} \\ c_{j\downarrow}^{\dagger}(1 - n_{j\uparrow}) & c_{j\downarrow}^{\dagger}c_{j\uparrow} & n_{j\downarrow}(1 - n_{j\uparrow}) & n_{j\downarrow}c_{j\uparrow} \\ -c_{j\downarrow}^{\dagger}c_{j\uparrow}^{\dagger} & -c_{j\downarrow}^{\dagger}n_{j\uparrow} & n_{j\downarrow}c_{j\uparrow}^{\dagger} & n_{j\downarrow}n_{j\uparrow} \end{pmatrix} (A.1)$$

The first row and column are deleted to obtain

$$\widetilde{Y} = \begin{pmatrix} (1 - n_{d,\downarrow}) n_{d,\uparrow} & -d_{\downarrow} d_{\uparrow}^{\dagger} & -d_{\downarrow} n_{d,\uparrow} \\ d_{\downarrow}^{\dagger} d_{\uparrow} & n_{d,\downarrow} (1 - n_{d,\uparrow}) & n_{d,\downarrow} d_{\uparrow} \\ -d_{\downarrow}^{\dagger} n_{d,\uparrow} & n_{d,\downarrow} d_{\uparrow}^{\dagger} & n_{d,\downarrow} n_{d,\uparrow} \end{pmatrix}.$$

Again one may identify $[m_j]_b^a = \left[\widetilde{X}_j\right]_b^a$, $[e_0]_a^b = \left[\widetilde{Y}\right]_a^b$, since eqs. (13b), (13a) are fulfilled.

The matrices X, \widetilde{X} are related by a particle-hole transformation, so that fermionization of H_h yields the same expression as in eq. (21). The fermionic representation of the impurity operator is denoted by \widetilde{H}_i :

$$\widetilde{H}_{i} = -\mu n_{d} + \frac{h}{2} \left(n_{d,\uparrow} - n_{d,\downarrow} \right) - 2DJ_{\alpha} n_{d,\uparrow} n_{d\downarrow} \left(\alpha + \widetilde{F}_{1,L} \right)$$

$$- DJ_{\alpha} \sqrt{\alpha} \sum_{\tau} \left[d_{\tau}^{\dagger} (1 - n_{d,\overline{\tau}}) (c_{L,\tau} + c_{1,\tau}) - d_{\tau} (1 - n_{d,\overline{\tau}}) (c_{L,\tau}^{\dagger} + c_{1,\tau}^{\dagger}) \right]$$

$$- DJ_{\alpha} \sum_{\tau} n_{d,\tau} \left(2n_{1,\overline{\tau}} + 2n_{L,\overline{\tau}} - c_{L,\overline{\tau}}^{\dagger} c_{1,\overline{\tau}} - c_{1,\overline{\tau}}^{\dagger} c_{L,\overline{\tau}} \right)$$

$$+ DJ_{\alpha} \sum_{\tau} d_{\tau}^{\dagger} d_{\overline{\tau}} \left(2c_{L,\overline{\tau}}^{\dagger} c_{L,\tau} + 2c_{1,\overline{\tau}}^{\dagger} c_{1,\tau} - c_{L,\overline{\tau}}^{\dagger} c_{1,\tau} - c_{1,\overline{\tau}}^{\dagger} c_{L,\tau} \right) + O\left(DJ_{\alpha} / \alpha^{1/2} \right) ,$$

where

$$2F_{1,L} = 2(n_1 + n_L) - c_{1,\uparrow}^{\dagger} c_{L,\uparrow} - c_{1,\downarrow}^{\dagger} c_{L,\downarrow} - c_{L,\uparrow}^{\dagger} c_{1,\uparrow} - c_{L,\downarrow}^{\dagger} c_{1,\downarrow} .$$

The canonical transformation generated by A, eq. (30), is also applicable to \widetilde{H}_i , and the doubly occupied state is energetically suppressed by scaling u_0 . In the Kondo limit, H_i and \widetilde{H}_i are seen to be identical.

Appendix A.2. gl(2|1)-symmetry

From the YBE (3), the direct product of two monodromy matrices is intertwined by an R-matrix,

$$(-1)^{p[\beta'](p[\alpha]+p[\alpha'])} \left[T^{(4,4)}(u) \otimes T^{(3,4)}(v) \right]_{\beta',\alpha'}^{\beta,\alpha} \left[R^{(3,4)}(v-u) \right]_{\alpha'',\beta''}^{\alpha',\beta'}$$

$$= \left[R^{(3,4)}(v-u) \right]_{\alpha',\beta'}^{\alpha,\beta} \left[T^{(3,4)}(v) \otimes T^{(4,4)}(u) \right]_{\alpha'',\beta''}^{\alpha',\beta'} (-1)^{p[\beta'](p[\alpha']+p[\alpha''])} . \quad (A.2)$$

The invariance of $\tau(u)$ with respect to gl(2|1) is shown by expanding eq. (A.2) in the limit $v \to \infty$, keeping only terms O(1), O(1/v).

$$R^{(3,4)}(v) \sim 1 + \frac{1}{v} \left(\frac{\alpha}{2} + 1 + (-1)^b e_a^b E_b^a \right) + \mathcal{O}\left(\frac{1}{v^2} \right)$$

$$T^{(3,4)}(v) =: R_{a,L}^{(3,4)}(v) R_{a,L-1}^{(3,4)}(v) \dots R_{a,0}^{(3,3)}(v + iu_0)$$

$$\sim 1 + \frac{1}{v} \left\{ \sum_{j=1}^{L} \left[\frac{\alpha}{2} + 1 + (-1)^b \left[e_a \right]_a^b \left[E_j \right]_b^a \right] + (-1)^b \left[e_a \right]_a^b \left[e_0 \right]_b^a \right\} + \mathcal{O}\left(\frac{1}{v^2} \right)$$

$$=: 1 + \frac{W}{v} + \mathcal{O}\left(\frac{1}{v^2} \right) .$$
(A.4)

 $T^{(4,4)}(u) \equiv T(u)$ is defined in eq. (16).

Eqs. (A.3), (A.4) are inserted into eq. (A.2) with d'' = 3; d = d' = 4, while keeping the full T(u). The constant terms on both sides are identical. In order O(1/v), one gets

$$\begin{split} (-1)^{p[\beta''](p[\alpha]+p[\alpha''])} [T(u)]^{\beta}_{\beta''} W^{\alpha}_{\alpha''} + [T(u)]^{\beta}_{\beta''} \left[(-1)^{p[a]p[b]} e^b_a E^a_b \right]^{\alpha,\beta'}_{\alpha'',\beta''} \\ &= (-1)^{p[\beta](p[\alpha]+p[\alpha''])} W^{\alpha}_{\alpha''} [T(u)]^{\beta}_{\beta''} + \left[(-1)^{p[a]p[b]} e^b_a E^a_b \right]^{\alpha,\beta}_{\alpha'',\beta'} [T(u)]^{\beta'}_{\beta''} \; . \end{split}$$

Set $\beta = \beta''$, multiply with $(-1)^{\beta}$ and sum over β . The second terms on each side are identical. The first terms give the commutator of the transfer matrix $\tau(u)$ with W:

$$\tau(u) := \sum_{\beta} (-1)^{\beta} [T(u)]_{\beta}^{\beta} , [\tau(u), W_{\alpha''}^{\alpha}] = 0 .$$
 (A.5)

Dropping constants in W, eq. (A.5) states that:

$$\left[\tau(u), \sum_{j=1}^{L} [E_j]_b^a + [e_0]_b^a\right] = 0.$$

Thus τ commutes with all global gl(2|1) symmetry operators. In a very similar way, one starts with eq. (10) to show

$$\left[\overline{\tau}(u), \sum_{j=1}^{L} [E_j]_b^a + [e_0]_b^a\right] = 0 ,$$

where $\overline{\tau}(u)$ is defined in eq. (17). Consequently, the Hamiltonian, defined by eq. (18), is gl(2|1)-symmetric.

Appendix B. Derivation of NLIE

The unknown functions in eqs. (40)-(44) are q_+ , q_- , $q_-^{(h)}$, $q_+^{(h)}$, where the indices pertain to two different sets of particle and hole solutions. Incidentally for the largest eigenvalue, the index denotes the part of the complex plane where these functions have zeroes: If a q- function carries an index + (-), it has zeroes in the upper (lower) half plane. From numerical studies for finite N, we know that in the largest eigenvalue case, the "particle solutions" obey $\mathrm{Im}[v_j] > 0$, $\mathrm{Im}[\tilde{v}_k] < 0 \ \forall j,k$. Analogously, the "hole solutions" are distributed in the complex plane as $\mathrm{Im}[v_j^{(h)}] < 1$, $\mathrm{Im}[\tilde{v}_k^{(h)}] > 1$, $\forall j,k$. The particle and hole solutions are distributed discretely and accumulate at certain points, prohibiting a formulation in terms of densities.

In the following, the largest eigenvalue case is studied. Consider the logarithmic derivative of these auxiliary functions, so that constant terms vanish. Since we know the analyticity properties of all functions in the complex v-plane, we can calculate their Fourier-transforms.

$$\hat{f} = \int_{-\infty}^{\infty} \left[\ln f(v)\right]' e^{-ikv} \frac{\mathrm{d}v}{2\pi} . \tag{B.1}$$

The integration contour is taken along the real axis. This is allowed as long as $|\alpha/2| > |u_N|$, which certainly is the case for N and α sufficiently large. \hat{f} vanishes

for k < 0 (k > 0) for f(v) analytic in \mathbb{C}^+ (\mathbb{C}^-) . Thus it is convenient to calculate the Fourier transforms separately for k < 0, k > 0. For the moment, concentrate on k < 0.

$$-\hat{\mathfrak{b}}(k) = -e^{(\alpha/2+1)k}\hat{\phi}_{-}(k) + e^{k}\hat{q}_{+}(k)$$
(B.2)

$$-\hat{\overline{\mathfrak{b}}}(k) = -e^{k\alpha/2}\hat{\phi}_{-}(k) - e^{k}\hat{q}_{+} + \hat{q}_{+}^{(h)}$$

$$-\hat{\mathfrak{c}}(k) = e^{k\alpha/2}(\hat{\phi}_{+}(k) - \hat{\phi}_{-}(k)) - e^{(\alpha/2+1)k}\phi_{-}(k) + \hat{\Lambda}_{i}(k)$$
(B.3)

$$-\hat{\mathbf{c}}(k) = e^{k\alpha/2}(\hat{\phi}_{+}(k) - \hat{\phi}_{-}(k)) - e^{(\alpha/2+1)k}\phi_{-}(k) + \hat{\Lambda}_{i}(k)$$
(B.4)

$$\hat{\mathfrak{B}}(k) = -e^k \hat{q}_+(k) + \hat{\Lambda}_i(k) \tag{B.5}$$

$$\hat{\overline{\mathfrak{B}}}(k) = \hat{q}_{+}(k) - \hat{q}_{+}^{(h)}(k) + \hat{\Lambda}_{i}(k)$$
(B.6)

$$\hat{\mathfrak{C}}(k) = -e^{k\alpha/2}\hat{\phi}_{+}(k) + \hat{q}_{+}^{(h)}(k) - \hat{\Lambda}_{i}(k) . \tag{B.7}$$

The essential observation is that in eqs. (B.2)-(B.7), there appear the three unknowns, namely \hat{q}_+ , $\hat{q}_+^{(h)}$ and $\hat{\Lambda}_i$, and the three auxiliary functions $\hat{\mathfrak{b}}$, $\hat{\overline{\mathfrak{b}}}$ and $\hat{\mathfrak{c}}$. Add eqs. (B.6), (B.7) and combine this sum with eq. (B.2):

$$\hat{\mathfrak{b}}(k) = e^{(\alpha/2+1)k} (\hat{\phi}_{-}(k) - \phi_{+}(k)) - e^{k} (\hat{\overline{\mathfrak{B}}}(k) + \hat{\mathfrak{C}}(k)) . \tag{B.8}$$

Combine eqs. (B.5) with (B.2) and these two with eq. (B.8). An expression for $\hat{\Lambda}_i$ results,

$$\hat{\Lambda}_i(k) = \hat{\mathfrak{B}}(k) + e^k(\hat{\overline{\mathfrak{B}}}(k) + \hat{\mathfrak{C}}(k)) + e^{(\alpha/2+1)k}\hat{\phi}_+(k) ,$$

which is inserted into eq. (B.4):

$$\hat{\mathfrak{c}}(k) = -e^{k\alpha/2}(\hat{\phi}_{+}(k) - \hat{\phi}_{-}(k)) + e^{(\alpha/2+1)k}(\hat{\phi}_{-}(k) - \hat{\phi}_{+}(k)) - \hat{\mathfrak{B}}(k) - e^{k}(\hat{\overline{\mathfrak{B}}}(k) + \hat{\mathfrak{C}}(k)).$$

Finally, eqs. (B.5) and (B.7) give $\hat{q}_{+}^{(h)}(k)$, which is inserted into eq. (B.3),

$$\hat{\overline{\mathfrak{b}}}(k) = e^{k\alpha/2}(\hat{\phi}_{-}(k) - \hat{\phi}_{+}(k)) - (\hat{\mathfrak{C}}(k) + \hat{\mathfrak{B}}(k)). \tag{B.9}$$

The case k > 0 is obtained by exchanging $\hat{\mathfrak{b}}$, $\hat{\overline{\mathfrak{b}}}$, switching $k \to -k$ in the exponential terms and replacing $\phi_- \leftrightarrow \phi_+$. The result is summarized:

$$\hat{\mathfrak{b}}(k) = \begin{cases} e^{-k\alpha/2} (\hat{\phi}_{+}(k) - \hat{\phi}_{-}(k)) - (\hat{\overline{\mathfrak{B}}}(k) + \hat{\mathfrak{C}}(k)) & k > 0 \\ -(\hat{\overline{\mathfrak{B}}}(k) + \hat{\mathfrak{C}}(k)) & k = 0 \\ e^{(\alpha/2+1)k} (\hat{\phi}_{-}(k) - \hat{\phi}_{+}(k)) - e^{k} (\hat{\overline{\mathfrak{B}}}(k) + \hat{\mathfrak{C}}(k)) & k < 0 \end{cases}$$

$$\hat{\overline{\mathfrak{b}}}(k) = \begin{cases} e^{-(\alpha/2+1)k} (\hat{\phi}_{+}(k) - \hat{\phi}_{-}(k)) - e^{-k} (\hat{\mathfrak{B}}(k) + \hat{\mathfrak{C}}(k)) & k > 0 \\ -(\hat{\mathfrak{B}}(k) + \hat{\mathfrak{C}}(k)) & k = 0 \\ e^{k\alpha/2} (\hat{\phi}_{-}(k) - \hat{\phi}_{+}(k)) - (\hat{\mathfrak{B}}(k) + \hat{\mathfrak{C}}(k)) & k < 0 \end{cases}$$

$$\hat{\mathfrak{c}}(k) = \begin{cases} (e^{-(\alpha/2+1)k} + e^{-k\alpha/2}) (\hat{\phi}_{+}(k) - \hat{\phi}_{-}(k)) - \hat{\overline{\mathfrak{B}}}(k) - e^{-k} (\hat{\mathfrak{B}}(k) + \hat{\mathfrak{C}}(k)) & k > 0 \\ -\hat{\overline{\mathfrak{B}}}(k) - (\hat{\mathfrak{B}}(k) + \hat{\mathfrak{C}}(k)) & k = 0 \end{cases}$$

$$\hat{\mathfrak{c}}(k) = \begin{cases} (e^{-(\alpha/2+1)k} + e^{-k\alpha/2}) (\hat{\phi}_{+}(k) - \hat{\phi}_{-}(k)) - \hat{\overline{\mathfrak{B}}}(k) - e^{-k} (\hat{\mathfrak{B}}(k) + \hat{\mathfrak{C}}(k)) & k > 0 \\ -\hat{\overline{\mathfrak{B}}}(k) - (\hat{\mathfrak{B}}(k) + \hat{\mathfrak{C}}(k)) & k = 0 \end{cases}$$

Application of the inverse Fourier transform and integration leads to a system of nonlinear integral equations.

$$\ln \mathfrak{b}(v) = \phi_{\mathfrak{b}}^{(N)}(v + \mathrm{i}\delta) - [k_{\mathfrak{b}} * \ln \overline{\mathfrak{B}}](v + 2\mathrm{i}\delta) - [k_{\mathfrak{b}} * \ln \mathfrak{C}](v + \mathrm{i}\delta) + \beta(\mu + h/2)$$
 (B.10)

$$\ln \overline{\mathfrak{b}}(v) = \phi_{\overline{\mathfrak{b}}}^{(N)}(v - \mathrm{i}\delta) - [k_{\overline{\mathfrak{b}}} * \ln \mathfrak{B}](v - 2\mathrm{i}\delta) - [k_{\overline{\mathfrak{b}}} * \ln \mathfrak{C}](v - \mathrm{i}\delta) + \beta(\mu - h/2)$$
(B.11)

$$\ln \mathfrak{c}(v) = \phi_{\mathfrak{c}}^{(N)}(v) - [k_{\mathfrak{b}} * \ln \overline{\mathfrak{B}}](v + \mathrm{i}\delta) - [k_{\overline{\mathfrak{b}}} * \ln \mathfrak{B}](v - \mathrm{i}\delta) - [k_{\mathfrak{c}} * \ln \mathfrak{C}](v) + 2\beta\mu , (B.12)$$

where the convolution

$$[f * g](x) := \int_{-\infty}^{\infty} f(x - y)g(y)dy$$
(B.13)

is done with local kernels:

$$k_{\mathfrak{b}}(v) = \frac{1}{2\pi v(v-\mathrm{i})}$$
, $k_{\overline{\mathfrak{b}}}(v) = k_{\mathfrak{b}}(v)^*$, $k_{\mathfrak{c}}(v) = k_{\mathfrak{b}}(v) + k_{\overline{\mathfrak{b}}}(v) = \frac{2}{2\pi(v^2+1)}$.

In order to achieve convergence, the equation for $\ln \mathfrak{b}$ ($\ln \overline{\mathfrak{b}}$), eq. (B.10) (eq. (B.11)), is taken for $v + i\delta$, ($v - i\delta$).

The constant terms are integration constants derived from the asymptotic behavior of the auxiliary functions for large |v|.

$$\lim_{|v| \to \infty} \mathfrak{b} = \frac{a}{1 + \overline{a}}, \lim_{|v| \to \infty} \overline{\mathfrak{b}} = \frac{\overline{a}}{1 + a}, \lim_{|v| \to \infty} \mathfrak{c} = \frac{a\overline{a}}{1 + a + \overline{a}}$$
(B.14)

$$a = e^{\beta(\mu + h/2)}, \ \overline{a} = e^{\beta(\mu - h/2)}.$$
 (B.15)

The inhomogeneities are

$$\phi_{\mathfrak{b}}^{(N)}(v) = \ln \frac{\phi_{+}\left(v + i\frac{\alpha}{2}\right) \phi_{-}\left(v - i\frac{\alpha}{2} - i\right)}{\phi_{-}\left(v + i\frac{\alpha}{2}\right) \phi_{+}\left(v - i\frac{\alpha}{2} - i\right)}$$

$$\phi_{\mathfrak{b}}^{(N)} = \left[\phi_{\mathfrak{b}}^{(N)}\right]^{*}$$

$$\phi_{\mathfrak{c}}^{(N)} = \phi_{\mathfrak{b}}^{(N)} + \phi_{\overline{\mathfrak{b}}}^{(N)}.$$

The thermodynamic limit $N \to \infty$ can be carried out leading to eqs. (45a)-(45c).

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